CANADIAN MATHEMATICAL SOCIETY SERIES OF MONOGRAPHS AND ADVANCED TEXTS

Monographies et Études de la Société Mathématique du Canada

EDITORIAL BOARD

Frederick V. Atkinson, Bernhard Banaschewski, Colin W. Clark, Erwin O. Kreyszig (Chairman) and John B. Walsh

Frank H. Clarke ***Optimization and Nonsmooth Analysis***

Erwin Klein and Anthony C. Thompson ***Theory of Correspondences: Including Applications to Mathematical Economics***

I. Gohberg, P. Lancaster, and L. Rodman ***Invariant Subspaces of Matrices with Applications***

Jonathan M. Borwein and Peter B. Borwein ***Pi and the AGM—A Study in Analytic Number Theory and Computational Complexity***

Pi and the AGM

A Study in Analytic Number Theory and Computational Complexity

JONATHAN M. BORWEIN

PETER B. BORWEIN

Department of Mathematics
Dalhousie University
Halifax, Nova Scotia

A Wiley-Interscience Publication

JOHN WILEY & SONS

New York • Chichester • Brisbane • Toronto • Singapore

To our mathematician father, David Borwein

Copyright © 1987 by John Wiley & Sons, Inc.

All rights reserved. Published simultaneously in Canada.

Reproduction or translation of any part of this work beyond that permitted by Section 107 or 108 of the 1976 United States Copyright Act without the permission of the copyright owner is unlawful. Requests for permission or further information should be addressed to the Permissions Department, John Wiley & Sons, Inc.

Library of Congress Cataloging-in-Publication Data:

Borwein, Jonathan M.
Pi and the AGM.

(Canadian Mathematical Society series of monographs and advanced texts = Monographies et études de la Société mathématique du Canada)
"A Wiley-Interscience publication."
Includes index.
1. Numbers, Theory of. 2. Computational complexity. 3. Functions, Elliptic. 4. Pi. I. Borwein, Peter B. II. Title. III. Series: Canadian Mathematical Society series of monographs and advanced texts.
QA241.B774 1986 512'.7 86-15811
ISBN 0-471-83138-7

Printed in the United States of America

10 9 8 7 6 5 4 3 2 1

Five thousand digits of pi.

3.

1415926535	8979323846	2643383279	5028841971	6939937510	5820974944	5923078164	0628620899	8628034825	3421170679
8214808651	3282306647	0938446095	5058223172	5359408128	4811174502	8410270193	8521105559	6446229489	5493038196
4428810975	6659334461	2847564823	3786783165	2712019091	4564856692	3460348610	4543266482	1339360726	0249141273
7245870066	0631558817	4881520920	9628292540	9171536436	7892590360	0113305305	4882046652	1384146951	9415116094
3305727036	5759591953	0921861173	8193261179	3105118548	0744623799	6274956735	1885752724	8912279381	8301194912
9833673362	4406566430	8602139494	6395224737	1907021798	6094370277	0539217176	2931767523	8467481846	7669405132
0005681271	4526356082	7785771342	7577896091	7363717872	1468440901	2249534301	4654958537	1050792279	6892589235
4201995611	2129021960	8640344181	5981362977	4771309960	5187072113	4999999837	2978049951	0597317328	1609631859
5024459455	3469083026	4252230825	3344685035	2619311881	7101000313	7838752886	5875332083	8142061717	7669147303
5982534904	2875546873	1159562863	8823537875	9375195778	1857780532	1712268066	1300192787	6611195909	2164201989
3809525720	1065485863	2788659361	5338182796	8230301952	0353018529	6899577362	2599413891	2497217752	8347913151
5574857242	4541506959	5082953311	6861727855	8890750983	8175463746	4939319255	0604009277	0167113900	9848824012
8583616035	6370766010	4710181942	9555961989	4676783744	9448255379	7747268471	0404753464	6208046684	2590694912
9331367702	8989152104	7521620569	6602405803	8150193511	2533824300	3558764024	7496473263	9141992726	0426992279
6782354781	6360093417	2164121992	4586315030	2861829745	5570674983	8505494588	5869269956	9092721079	7509302955
3211653449	8720275596	0236480665	4991198818	3479775356	6369807426	5425278625	5181841757	4672890977	7727938000
8164706001	6145249192	1732172147	7235014144	1973568548	1613611573	5255213347	5741849468	4385233239	0739414333
4547762416	8625189835	6948556209	9219222184	2725502542	5688767179	0494601653	4668049886	2723279178	6085784383
8279679766	8145410095	3883786360	9506800642	2512520511	7392984896	0841284886	2694560424	1965285022	2106611863
0674427862	2039194945	0471237137	8696095636	4371917287	4677646575	7396241389	0865832645	9958133904	7802759009
9465764078	9512694683	9835259570	9825822620	5224894077	2671947826	8482601476	9909026401	3639443745	5305068203
4962524517	4939965143	1429809190	6592509372	2169646151	5709858387	4105978859	5977297549	8930161753	9284681382
6868386894	2774155991	8559252459	5395943104	9972524680	8459872736	4469584865	3836736222	6260991246	0805124388
4390451244	1365497627	8079771569	1435997700	1296160894	4169486855	5848406353	4220722258	2848864815	8456028506
0168427394	5226746767	8895252138	5225499546	6672782398	6456596116	3548862305	7745649803	5593634568	1743241125
1507606947	9451096596	0940252288	7971089314	5669136867	2287489405	6010150330	8617928680	9208747609	1782493858
9009714909	6759852613	6554978189	3129784821	6829989487	2265880485	7564014270	4775551323	7964145152	3746234364
5428584447	9526586782	1051141354	7357395231	1342716610	2135969536	2314429524	8493718711	0145765403	5902799344
0374200731	0578539062	1983874478	0847848968	3321445713	8687519435	0643021845	3191048481	0058706146	8067491927
8191197939	9520614196	6342875444	0643745123	7181921799	9839101591	9561814675	1426912397	4894090718	6494231961
5679452080	9514655022	5231603881	9301420937	6213785595	6638937787	0830390697	9207734672	2182562599	6615014215
0306803844	7734549202	6054146659	2520149744	2850732518	6660021324	3408819071	0486331734	6496514539	0579626856
1005508106	6587969981	6357473638	4052571459	1028970641	4011097120	6280439039	7595156771	5770042033	7869936007
2305587631	7635942187	3125147120	5329281918	2618612586	7321579198	4148488291	6447060957	5270695722	0917567116
7229109816	9091528017	3506712748	5832228718	3520935396	5725121083	5791513698	8209144421	0067510334	6711031412
6711136990	8658516398	3150197016	5151168517	1437657618	3515565088	4909989859	9823873455	2833163550	7647918535
8932261854	8963213293	3089857064	2046752590	7091548141	6549859461	6371802709	8199430992	4488957571	2828905923
2332609729	9712084433	5732654893	8239119325	9746366730	5836041428	1388303203	8249037589	8524374417	0291327656
1809377344	4030707469	2112019130	2033038019	7621101100	4492932151	6084244485	9637669838	9522868478	3123552658
2131449576	8572624334	4189303968	6426243410	7732269780	2807318915	4411010446	8232527162	0105265227	2111660396
6655730925	4711055785	3763466820	6531098965	2691862056	4769312570	5863566201	8558100729	3606598764	8611791045
3348850346	1136576867	5324944166	8039626579	7877185560	8455296541	2665408530	6143444318	5867697514	5661406800
7002378776	5913440171	2749470420	5622305389	9456131407	1127000407	8547332699	3908145466	4645880797	2708266830
6343285878	5698305235	8089330657	5740679545	7163775254	2021149557	6158140025	0126228594	1302164715	5097925923
0990796547	3761255176	5675135751	7829666454	7791745011	2996148903	0463994713	2962107340	4375189573	5961458901
9389713111	7904297828	5647503203	1986915140	2870808599	0480109412	1472213179	4764777262	2414254854	5403321571
8530614228	8137585043	0633217518	2979866223	7172159160	7716692547	4873898665	4949450114	6540628433	6639379003
9769265672	1463853067	3609657120	9180763832	7166416274	8888007869	2560290228	4721040317	2118608204	1900042296
6171196377	9213375751	1495950156	6049631862	9472654736	4252308177	0367515906	7350235072	8354056704	0386743513
6222247715	8915049530	9844489333	0963408780	7693259939	7805419341	4473774418	4263129860	8099888687	4132604721

From the eleventh iteration of

$$x_{n+1} := (x_n^{1/2} + x_n^{-1/2})/2 \qquad x_0 := 2^{1/2}$$

$$y_{n+1} := (y_n x_n^{1/2} + x_n^{-1/2})/(y_n + 1) \qquad y_1 := 2^{1/4}$$

$$\pi_n := \pi_{n-1}(x_n + 1)/(y_n + 1) \qquad \pi_0 := 2 + 2^{1/2}$$

Preface

When I was a student, abelian functions were, as an effect of the Jacobian tradition, considered the uncontested summit of mathematics and each of us was ambitious to make progress in this field. And now? The younger generation hardly knows abelian functions.

How did this happen? In mathematics, as in other sciences, the same processes can be observed again and again. First, new questions arise, for internal or external reasons, and draw researchers away from the old questions. And the old questions, just because they have been worked on so much, need ever more comprehensive study for their mastery. This is unpleasant, and so one is glad to turn to problems that have been less developed and therefore require less foreknowledge—even if it is only a matter of axiomatics, or set theory, or some such thing.

And so there is nothing for it but to collect together the old subjects in good references... so that later developments may continue them, if fate should so decree.

Felix Klein (1849–1925) [79 p. 294]

A central thread of this book is the arithmetic-geometric mean iteration of Gauss, Lagrange, and Legendre. A second thread is the calculation of π. The two threads are intimately interwoven and provide a remarkable example of the application to twentieth-century computational concerns of the type of nineteenth-century analysis whose neglect Klein so deplores. The calculation of digits of π has had a fascination that has far exceeded utilitarian concerns—a fascination that has driven some to dedicate their lives to calculations we may now electronically effect in seconds. The methods that make the computation of hundreds of millions of digits of π or any elementary function within our grasp are rooted in the AGM and this is where our interest in the material began. Making sense of this material took us in three directions and motivated our writing this book.

The first direction leads to nineteenth-century analysis and in particular the transformation theory of elliptic integrals. This necessitates at least a brief discussion of a number of topics including elliptic integrals and functions, theta functions, and modular functions. These attractive and once central concerns of analysis have been dropped from the standard curriculum—and much that is beautiful has become relatively inaccessible except to the expert or the archivist. In presenting this material we have not striven for generality. This is available in the specialty literature. At times we have settled for giving only a taste of the material and a few pointers on where it can be pursued.

We have found this excuse to consult the nineteenth-century masters a pleasurable and rewarding bonus—as Hermann points out in his introduction to Klein [79], "We are so used to thinking in terms of the 'progress' of science that it is hard for us to remember that certain matters were better understood one hundred years ago."

The second direction takes us into the domain of analytic complexity. How intrinsically difficult is it to calculate algebraic functions, elementary functions and constants, and the familiar functions of mathematical physics? Here part of the attraction is the surprising answers—the familiar methods are often far from optimal.

Finally, an honest treatment invites exploration of applications and ancillary material, particularly the rich and beautiful interconnections between the function theory and the number theory. Included, for example, are the Rogers–Ramanujan identities; algebraic series for π; results on sums of two and four squares; the transcendence of π and e; and a discussion of Madelung's constant, lattice sums, and elliptic invariants.

Our primary concern throughout has been the interplay of analysis and mathematical application. We hope we have elucidated a variety of useful and attractive analytic techniques. This book should be accessible to any graduate student. Only rarely does it assume more than the content of undergraduate courses in real and complex analysis. It is, however, at times terse, at times computational, and some of the exercises are difficult. A fair amount of the material, particularly on the approximation and computation of π and the elementary functions, is new and only partially available in research papers.

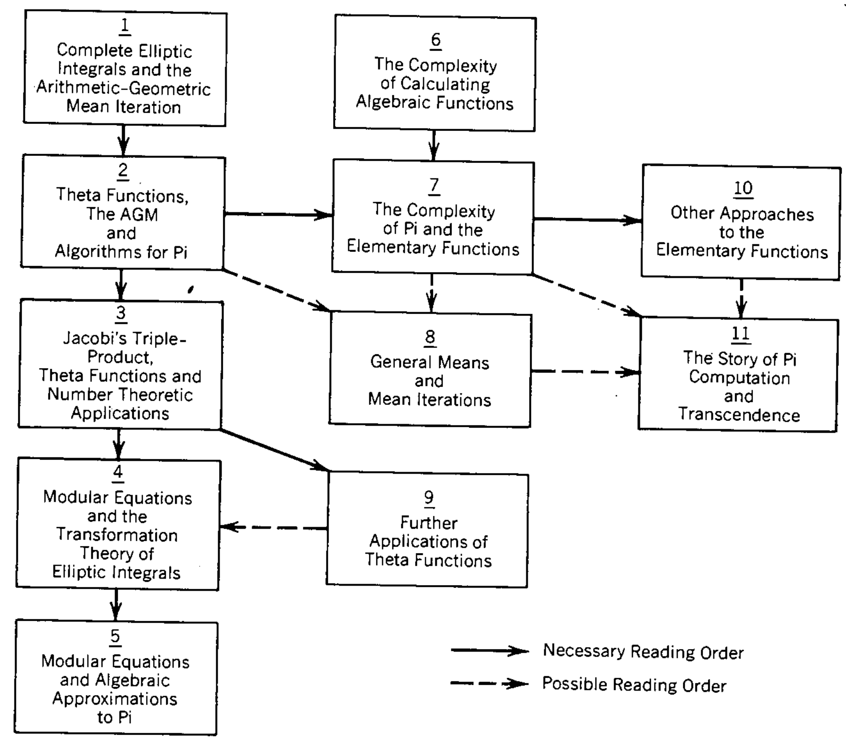
The accompanying flow-chart gives possible routes through the material. Chapters 8 and 11 are largely self-contained. Chapter 8 is a treatment of general mean iterations, while Chapter 11 sketches some of the history of pi, its calculation and its transcendence. There are numerous exercises (frequently with hints). The exercises often develop substantial additional examples and bodies of theory, and even the casual reader is encouraged to look at them.

The contributions of family, friends, students, and colleagues have been many and varied and have greatly facilitated the production of this book. To all these people we offer our thanks. A particular debt of gratitude is owed to Professors R. Askey, B. Berndt, R. Brent, K. Dilcher, W. Gosper, Y. Kanada, D. Shanks, and J. Zucker. Their thoughtful comments and sugges-

tions helped produce a better book. The cheerful technical assistance of P. Flemming, of our departmental office, and of the staff at Wiley is also gratefully acknowledged, as is the assistance of the Canadian Mathematical Society and the support of the Natural Sciences and Engineering Research Council of Canada.

Jonathan M. Borwein
Peter B. Borwein

Halifax, Nova Scotia
November 1986



Biographical Information

Jonathan M. Borwein was born in St. Andrews Scotland in 1951. In 1971 he obtained an Honours B.Sc. in mathematics from the University of Western Ontario, where his father is still head of the mathematics department. He was awarded an Ontario Rhodes Scholarship that year which he held at Jesus College Oxford, where he was awarded a mathematics D.Phil. in 1974 under the supervision of Michael Dempster. Since then he has been on the faculty of Dalhousie University and has been Professor of Mathematics since 1984. He has also been on faculty at Carnegie-Mellon University (1980–1982) and has spent visiting research periods at Cambridge, Limoges, and the University of Montreal. His other research interests are in classical analysis, functional analysis, and optimization theory.

Peter B. Borwein was born in St. Andrews Scotland in 1953. He obtained an Honours B.Sc. in mathematics from the University of Western Ontario in 1974, and a Ph.D, under the supervision of David Boyd, from the University of British Columbia in 1979. He spent 1979–1980 as a NATO research fellow in Oxford. Since then he has been a faculty member at Dalhousie University and is now Associate Professor of Mathematics. He has spent a sabbatical year at the University of Toronto. His other research interests are in approximation theory, classical analysis, and geometry.

Contents

Chapter One

Complete Elliptic Integrals and the Arithmetic-Geometric Mean Iteration

Abstract. *The focus of this chapter is the arithmetic-geometric mean (AGM) iteration of Gauss, Lagrange, and Legendre and its relationship to elliptic integrals. The iteration converges quadratically to a nonelementary transcendental function simply expressible in terms of complete elliptic integrals. This result, which is fundamental to this monograph, is established in a variety of ways. Some of the basic properties of elliptic integrals and functions are discussed.*

1.1 *THE ARITHMETIC-GEOMETRIC MEAN ITERATION*

One of the jewels of classical analysis is the *arithmetic-geometric mean* (AGM) iteration of Gauss. It is the following two-term recursion:

(1.1.1) $$a_{n+1} := \frac{a_n + b_n}{2}$$

(1.1.2) $$b_{n+1} := \sqrt{a_n b_n}\,.$$

It is customary and useful to introduce an auxiliary variable,

(1.1.3) $$c_{n+1} := \tfrac{1}{2}(a_n - b_n)\,.$$

If we assume that $0 < b_0 \leq a_0$, then from the arithmetic-geometric mean inequality we have

$$b_n \le b_{n+1} \le a_{n+1} \le a_n$$

and

$$0 \le a_{n+1} - b_{n+1} = \frac{1}{2} \frac{(a_n - b_n)^2}{(\sqrt{a_n} + \sqrt{b_n})^2} . \tag{1.1.4}$$

Whence we observe that a_n and b_n converge to a common limit determined uniquely by a_0 and b_0. This common limit will be denoted (on letting $a := a_0$ and $b := b_0$) by

$$M(a, b) := \lim_{n\to\infty} a_n = \lim_{n\to\infty} b_n . \tag{1.1.5}$$

We will refer to this limiting process as the AGM and usually reserve the symbols a_n, b_n, and c_n for variables bound by the AGM relations. We also reserve the symbol AG(a, b) for the common limit.

We say that $\alpha_n \to \alpha$ with pth-order convergence if

$$\left| \frac{\alpha_{n+1} - \alpha}{(\alpha_n - \alpha)^p} \right| = O(1) \tag{1.1.6}$$

where, as usual, $\alpha_n = O(\beta_n)$ means that, for some constant c and for all n, $\alpha_n \le c\beta_n$. If the α_n are functions defined for all x in a set K, and if the implicit constant concealed by the O symbol in (1.1.6) is independent of x, then we say that the convergence is *uniformly* p*th order*. Roughly speaking, *quadratic* (second-order) convergence doubles the number-of-digits agreement between successive iterates and the limit, *cubic* (third-order) convergence triples the agreement, and so on.

It is an easy observation from (1.1.4) that the AGM converges uniformly quadratically for a_0, b_0 restricted to compact subsets of $(0, \infty)$. Very precise estimates for the rate of convergence will be established later.

We also observe that $M(a, b)$ is homogeneous, that is, for $\lambda > 0$

$$\lambda M(a, b) = M(\lambda a, \lambda b) \tag{1.1.7}$$

and thus there is little loss of generality, though often some loss of symmetry, to setting $a = 1$.

The function M satisfies

$$M(a, b) = M\left(\frac{a+b}{2}, \sqrt{ab}\right) \tag{1.1.8}$$

or

$$M(1, b) = \frac{1+b}{2} M\left(1, \frac{2\sqrt{b}}{1+b}\right) . \tag{1.1.9}$$

The analysis of the limit of the AGM rests on finding a two-variable function M invariant under the transformation (1.1.8) or, equivalently, on finding a function f satisfying the functional relation (1.1.9), namely,

$$f(x) = \frac{1+x}{2} f\left(\frac{2\sqrt{x}}{1+x}\right) . \tag{1.1.10}$$

If we set $k_0 := x \in (0, 1)$ and

$$k_{n+1} := \frac{2\sqrt{k_n}}{1+k_n} \tag{1.1.11}$$

then since

$$1 - k_{n+1} = \frac{(1-k_n)^2}{(1+\sqrt{k_n})^2(1+k_n)}$$

we have that $k_n \to 1$ quadratically. In fact, the function g defined by

$$g(x) := a \prod_{n=0}^{\infty} \frac{1+k_n}{2} \qquad k_0 := x \tag{1.1.12}$$

is the unique solution of (1.1.10) analytic in a neighbourhood of 1 that satisfies $g(1) = a$. (See Exercise 4.) This form of the AGM, as a single variable iteration, is usually called the *Legendre form*.

It is convenient and standard to define the *complement* x' of x by $x' := \sqrt{1-x^2}$. Differentiation will be denoted by $\dot{f}$.

Comments and Exercises

The early history of transformations of elliptic integrals, of which, as we shall see in the next section, the AGM is an example, is laid out in an entertaining article by G. N. Watson [33] entitled "The Marquis and the Land-Agent: A Tale of the Eighteenth Century." The marquis is Fagnano and the land-agent is Landen. Landen's transformation, published in 1775, will be discussed later. The names of Euler and Lagrange should also be associated with the early transformation theory. Lagrange uncovered the AGM iteration sometime before 1785. Gauss rediscovered it independently in the 1790s. He apparently first considered the iteration in 1791 at the age of 14 (Almquist and Berndt [Pr]). It is, however, Gauss and Legendre who develop the theory fully. As Watson [33] points out, "in the hands of Legendre, the transformation became a most powerful method for computing elliptic integrals." Gauss is unique in having deduced the invariant function from the functional equation rather than proceeding in the opposite (and easier) direction.

1. Deduce that, for the AGM,

$$a_n = a_{n+1} + c_{n+1} \qquad b_n = a_{n+1} - c_{n+1} \qquad c_n^2 = a_n^2 - b_n^2 .$$

Hence the AGM is well defined for negative n. Show that

$$a_{-n} = 2^n a_n^* \qquad b_{-n} = 2^n c_n^* \qquad c_{-n} = 2^n b_n^* ,$$

where a_n^*, b_n^* and c_n^* are generated from the AGM commencing with $a_0^* := a_0$, $b_0^* := c_0$, and $c_0^* := b_0$. Show that

$$c_n = \frac{c_{n-1}^2}{4a_n} .$$

Observe that this formula avoids the subtractive cancellation problems inherent in calculating the very small number c_n from $c_{n+1} = \frac{1}{2}(a_n - b_n)$. Show that

$$a_{n+1} = \frac{a_n + \sqrt{a_{n-1}(2a_n - a_{n-1})}}{2} .$$

2. Consider the *harmonic-geometric mean* iteration

$$\alpha_{n+1} := \frac{2\alpha_n\beta_n}{\alpha_n + \beta_n}$$

$$\beta_{n+1} := \sqrt{\alpha_n\beta_n} .$$

Show, for $\alpha_0, \beta_0 \in (0, \infty)$, that the above iteration converges quadratically to $H(\alpha_0, \beta_0)$, where

$$H(\alpha_0, \beta_0) = \frac{1}{M(1/\alpha_0, 1/\beta_0)} .$$

3. Consider the *arithmetic-harmonic mean* iteration

$$\alpha_{n+1} := \frac{\alpha_n + \beta_n}{2}$$

$$\beta_{n+1} := \frac{2\alpha_n\beta_n}{\alpha_n + \beta_n} .$$

Show, for $\alpha_0, \beta_0 \in (0, \infty)$, that the above iteration converges quadratically and that

$$\lim \alpha_n = \lim \beta_n = \sqrt{\alpha_0\beta_0} .$$

4. Show that the AGM is a well-defined quadratically convergent iteration for starting values $a_0 := 1$, $b_0 := z$, where $\mathrm{re}(z) > 0$. Likewise the function g of (1.1.12) is a single-valued analytic function on $\mathrm{re}(z) > 0$. In both cases the convergence is uniformly quadratic on compact subsets. [The root must always be chosen to lie in $\mathrm{re}(z) > 0$.] Show that $g(z) = M(1, z)$ for $\mathrm{re}(z) > 0$.

1.2 *GAUSS'S DERIVATION OF THE FUNDAMENTAL LIMIT FORMULA*

By May 30th, 1799, Gauss had observed, purely computationally, that

$$(1.2.1) \qquad \frac{1}{M(1, \sqrt{2})} \quad \text{and} \quad \frac{2}{\pi}\int_0^1 \frac{dt}{\sqrt{1 - t^4}}$$

agreed to at least eleven decimal places. He commented in his diary that this result "will surely open up a whole new field of analysis"—a claim vindicated by the subsequent directions of nineteenth-century mathematics. The inverse of the above (indefinite) integral is the lemniscate sine, a function Gauss studied in some detail. He had recognized it as a doubly periodic function (see Section 1.7) by the year 1800 and hence had anticipated one of the most important developments of Abel and Jacobi: the inversion of algebraic integrals.

We now outline Gauss's derivation of the limit of the AGM (Gauss [1866]). This is not the easiest development but it may be the most motivated.

Theorem 1.1

$$\frac{1}{M(1, x)} = \frac{2}{\pi}\int_0^{\pi/2} \frac{d\theta}{\sqrt{1 - (1 - x^2)\sin^2\theta}} .$$

First proof. Observe that $[M(1 + x, 1 - x)]^{-1}$, defined by (1.1.5), is analytic and even in some neighbourhood of zero. (See Exercise 4, Section 1.) Thus we may suppose that

$$(1.2.2) \qquad \frac{1}{M(1 + x, 1 - x)} = 1 + d_1x^2 + d_2x^4 + d_3x^6 + \cdots .$$

Upon application of the AGM transformation we have

$$(1.2.3) \qquad \frac{1}{M(1 + 2\sqrt{x}/(1 + x), 1 - 2\sqrt{x}/(1 + x))} = \frac{1}{M(1, \sqrt{1 - 4x/(1 + x^2)})} = \frac{1 + x}{M(1 + x, 1 - x)} .$$

Comparing (1.2.2) and (1.2.3) gives

$$(1+x)(1+d_1x^2+d_2x^4+\cdots)=1+d_1\left(\frac{2\sqrt{x}}{1+x}\right)^2+d_2\left(\frac{2\sqrt{x}}{1+x}\right)^4+\cdots. \tag{1.2.4}$$

We leave it as an exercise to the reader to follow Gauss's footsteps by solving the above equation for d_i. In fact,

$$d_i=\left[\frac{(2i-1)!}{i!(i-1)!}\right]^2\frac{1}{4^{2i-1}}. \tag{1.2.5}$$

If we observe, as in (1.2.3), that

$$\frac{1}{M(1,\sqrt{1-x^2})}=\frac{1}{M(1+x,1-x)} \tag{1.2.6}$$

we see by (1.2.2) that we are finished if we show that

$$\frac{2}{\pi}\int_0^{\pi/2}\frac{d\theta}{\sqrt{1-x^2\sin^2\theta}}=\sum_{i=0}^{\infty}\left[\frac{(2i-1)!}{i!(i-1)!}\right]^2\frac{x^{2i}}{4^{2i-1}} \tag{1.2.7}$$

This final equation requires expanding $(1-x^2\sin^2\theta)^{-1/2}$ and integrating term by term.

It is perhaps possible to be guided to the limit of the AGM by the above method. If, however, one has correctly guessed the limit, then proving it correct is much more straightforward and only involves establishing the invariance of the limit under the transformation.

Second proof. Let

$$T(a,b):=\frac{2}{\pi}\int_0^{\pi/2}\frac{d\theta}{\sqrt{a^2\cos^2\theta+b^2\sin^2\theta}}. \tag{1.2.8}$$

Then, as the substitution $t:=b\tan\theta$ shows,

$$T(a,b)=\frac{1}{\pi}\int_{-\infty}^{\infty}\frac{dt}{\sqrt{(a^2+t^2)(b^2+t^2)}}. \tag{1.2.9}$$

Now the substitution $u:=\frac{1}{2}(t-ab/t)$ (and some care) yields

$$T(a,b)=T\left(\frac{a+b}{2},\sqrt{ab}\right). \tag{1.2.10}$$

It follows that $T(a_n,b_n)$ is independent of n and hence, since (1.2.9) evaluates as an arctan when $a=b$, we have on interchanging limit and integration

$$T(a_0,b_0)=T(M(a_0,b_0),M(a_0,b_0))=\frac{1}{M(a_0,b_0)}. \quad \square \tag{1.2.11}$$

Comments and Exercises

An excellent account of the development and the importance of elliptic function theory in the nineteenth century is to be found in Felix Klein's classical work, "Development of Mathematics in the 19th Century" (Klein [79]). Gauss's works are, of course, available in collected form (Gauss [1866]). Before establishing the limit formula, Gauss produces partial expansions of $M(1,x)$ and $M(1+x,1-x)$ plus a number of AGM calculations carried to as many as 20 decimals. It is apparent that both the observation of the limit and the route to a proof were indicated by prodigious numerical experimentation.

The second proof may be found in Carlson [71], Newman [82, 85], Todd [79], or Wimp [84]. Carlson [71] offers some interesting generalizations. These are discussed in Section 8.5.

1. Fill in the details in the above proofs. In particular prove (1.2.5), (1.2.7), and (1.2.10).

2. Show that $[M(1+x,1-x)]^{-1}$ and $[M(1,x)]^{-1}$ both solve the second-order differential equation

$$(x^3-x)\frac{d^2y}{dx^2}+(3x^2-1)\frac{dy}{dx}+xy=0.$$

Hint: For the second solution consider equation (1.2.6).

1.3 *BASIC PROPERTIES OF COMPLETE ELLIPTIC INTEGRALS*

The two basic integrals we will encounter are the *complete elliptic integral of the first kind*,

$$K(k):=\int_0^{\pi/2}\frac{d\theta}{\sqrt{1-k^2\sin^2\theta}} \tag{1.3.1}$$

$$=\int_0^1\frac{dt}{\sqrt{(1-t^2)(1-k^2t^2)}}$$

and the *complete elliptic integral of the second kind*, (1.3.2) $$E(k) := \int_0^{\pi/2} \sqrt{1-k^2\sin^2\theta}\,d\theta = \int_0^1 \frac{\sqrt{1-k^2t^2}}{\sqrt{1-t^2}}\,dt\,.$$

The *complementary integrals* E' and K' are the integrals in the complementary variable $k' = \sqrt{1-k^2}$,

(1.3.3) $$K'(k) := K(\sqrt{1-k^2}) = K(k')$$

(1.3.4) $$E'(k) := E(\sqrt{1-k^2}) = E(k')\,.$$

As is traditional, we will use the notation $f'(k) := f(k')$ to indicate any function in the complementary variable. The variable k is often called the *modulus*, and k' is the *complementary modulus*.

The second integral arises in the rectification of ellipses. The arc-length A of an ellipse with semiaxes a and b is given by

$$A = 4\int_0^{\pi/2} \sqrt{a^2\cos^2\theta + b^2\sin^2\theta}\,d\theta = 4aE'\left(\frac{b}{a}\right).$$

The first integral has the following physical interpretation. If p is the period of a pendulum with amplitude α and length L, then

$$p = 4\sqrt{\frac{L}{g}}\,K\left(\sin\left(\frac{\alpha}{2}\right)\right)$$

where g is the gravitational constant. Note as $\alpha \to 0$, $K(\sin(\alpha/2)) \to \pi/2$, and we are left with a simple harmonic approximation.

The Gaussian hypergeometric series, discussed by Gauss in 1812 in what is one of the first rigorous discussions of convergent series, is defined by

(1.3.5) $$F(a, b; c; z) := 1 + \frac{a\cdot b}{1\cdot c}z + \frac{a(a+1)b(b+1)}{1\cdot 2\cdot c(c+1)}z^2 + \frac{a(a+1)(a+2)b(b+1)(b+2)}{1\cdot 2\cdot 3\cdot c(c+1)(c+2)}z^3 + \cdots.$$

For the complete elliptic integrals we have the series expansions, for $|k| < 1$,

(1.3.6) $$K(k) = \frac{\pi}{2}\sum_{i=0}^{\infty}\left[\frac{(2i-1)!!}{2^i i!}\right]^2 k^{2i} = \frac{\pi}{2}F\left(\frac{1}{2}, \frac{1}{2}; 1; k^2\right)$$

(1.3.7) $$E(k) = \frac{\pi}{2}\left\{1 - \sum_{i=1}^{\infty}\left[\frac{(2i-1)!!}{2^i i!}\right]^2 \frac{k^{2i}}{2i-1}\right\} = \frac{\pi}{2}F\left(-\frac{1}{2}, \frac{1}{2}; 1; k^2\right)$$

where $(2i-1)!! := 1\cdot 3\cdot 5\cdots(2i-1)$. The derivations are left as Exercise 1.

We have, as in Exercise 2 of Section 1.2, that K and K' are both solutions of

(1.3.8) $$(k^3 - k)\frac{d^2y}{dk^2} + (3k^2 - 1)\frac{dy}{dk} + ky = 0\,.$$

This equation has a regular singular point at zero (the roots of the indicial equation are both 0) which, as the reader familiar with the elementary theory of second-order differential equations knows, says that

(1.3.9) $$K'(k) = a\log k\,K(k) + f(k)$$

where f is analytic in a neighbourhood of zero. (See, for example, Birkhoff and Rota [69].)

In fact,

(1.3.10) $$K'(k) = \frac{2}{\pi}\log\left(\frac{4}{k}\right)K(k) - 2\left[\left(\frac{1}{2}\right)^2\left(\frac{1}{1\cdot 2}\right)k^2 + \left(\frac{1\cdot 3}{2\cdot 4}\right)^2\left(\frac{1}{1\cdot 2} + \frac{1}{3\cdot 4}\right)k^4 + \left(\frac{1\cdot 3\cdot 5}{2\cdot 4\cdot 6}\right)^2\left(\frac{1}{1\cdot 2} + \frac{1}{3\cdot 4} + \frac{1}{5\cdot 6}\right)k^6 + \cdots\right].$$

This logarithmic asymptote at zero will be of considerable interest later in the discussion of the complexity of log. Also,

(1.3.11) $$E'(k) = 1 + \frac{1}{2}\left[\log\left(\frac{4}{k}\right) - \frac{1}{1\cdot 2}\right]k^2 + \left(\frac{1^2\cdot 3}{2^2\cdot 4}\right)\left[\log\left(\frac{4}{k}\right) - \frac{2}{1\cdot 2} - \frac{1}{3\cdot 4}\right]k^4 + \left(\frac{1^2\cdot 3^2\cdot 5}{2^2\cdot 4^2\cdot 6}\right)\left[\log\left(\frac{4}{k}\right) - \frac{2}{1\cdot 2} - \frac{2}{3\cdot 4} - \frac{1}{5\cdot 6}\right]k^6 + \cdots.$$

Once again the above verifications are left as exercises.

The first and second integrals are linked by the equations

(1.3.12) $$\frac{dE}{dk} = \frac{E-K}{k}$$

(1.3.13) $$\frac{dK}{dk} = \frac{E - k'^2K}{k(k')^2}\,.$$

(See Exercises 2 and 3.)

Comments and Exercises

The functions K and E are nonelementary transcendental functions. This is a result of Liouville's. In general an elliptic integral is an integral of the form

$$\int^u R(x, y)\, dx ,$$

where R is a rational function of x and y and where y^2 is a quartic polynomial in x. Except in special cases, such as repeated factors, this is always a nonelementary function of u. Incomplete elliptic integrals of the third kind are of the form

$$\int_0^u \frac{dx}{(1-\eta x^2)\sqrt{(1-x^2)(1-k^2x^2)}} .$$

The integral is complete when $u = 1$. (The complete third integral can be expressed in terms of K and E.) Analogously we may define incomplete elliptic integrals of the first and second kind. The basic result due to Legendre is that any elliptic integral may be algebraically reduced to a linear combination of elliptic integrals of the first, second, and third kind. (See also Exercise 5 of Section 1.4 and Exercise 6 of Section 1.6.)

The formulae in the section may be found, in tabular form, in Abramowitz and Stegun [64], Gradshteyn and Ryzhik [80], and the Bateman project (Erdélyi et al. [53]), so may transformation formulae for the hypergeometric functions. Of course the indispensible companion volume is Whittaker and Watson [27].

A number of the seminal nineteenth-century papers, including Gauss's on the hypergeometric series and Jacobi's on theta functions, are available in translation in Birkhoff [73].

1. Establish the series expansions (1.3.6) and (1.3.7) for K and E by expanding the radical by the binomial theorem and integrating term by term.
2. Establish, by differentiating the integral (1.3.2), that

$$\frac{dE}{dk} = \frac{E-K}{k} .$$

3. Verify, from the series expansions (1.3.6) and (1.3.7), that

$$\frac{dK}{dk} = \frac{E-k'^2K}{kk'^2} .$$

4. From the integral representations show that

a) $K(0) = \frac{\pi}{2} \qquad E(0) = \frac{\pi}{2} \qquad E(1) = 1 .$

b) $K'(k) = \log\left(\frac{4}{k}\right) + 0(k^2|\log k|) \qquad k \downarrow 0 .$

Hint:

$$\int_0^{\pi/2} \frac{d\theta}{\sqrt{1-(1-k^2)\sin^2\theta}} = \int_0^{\pi/2} \frac{k' \sin\theta\, d\theta}{\sqrt{k^2+(k')^2\cos^2\theta}} + \int_0^{\pi/2} \sqrt{\frac{1-k'\sin\theta}{1+k'\sin\theta}}\, d\theta .$$

The second integral evaluates to $\log[(1+k')/k]$. (See Borwein and Borwein [84a].)

c) $\left|K'(k) - \log\left(\frac{4}{k}\right)\right| \le 4k^2(8+|\log k|) \qquad k \in (0, 1]$.

5. Verify the expansions (1.3.10) and (1.3.11). (See also Exercise 1, Section 2.3.)
6. Establish the relation, for $\mathrm{re}(c) > \mathrm{re}(b) > 0$,

$$F(a, b; c; z) = C\int_0^1 t^{b-1}(1-t)^{c-b-1}(1-tz)^{-a}\, dt$$

where C is a constant independent of z. [In fact $C = \Gamma(c)/\Gamma(b)\Gamma(c-b)$ where, as usual, Γ is the gamma function. (See Section 1.6.)] Note that this provides an analytic continuation of F to $\mathbb{C} - [1, \infty)$.

7. Show that $F(a, b; c; z)$ satisfies

$$z(1-z)\frac{d^2y}{dz^2} + [c-(a+b+1)z]\frac{dy}{dz} - aby = 0 .$$

This is the *hypergeometric differential equation.*

1.4 *QUADRATIC TRANSFORMATIONS AND ITERATIONS AND A THIRD PROOF OF THE FUNDAMENTAL LIMIT FORMULA*

The complete elliptic integrals satisfy the following functional relations which we collect together as

Theorem 1.2

For $k \in (0,1)$,

(a) $K(k) = \dfrac{1}{1+k} K\left(\dfrac{2\sqrt{k}}{1+k}\right)$ (upward)

(b) $K(k) = \dfrac{2}{1+k'} K\left(\dfrac{1-k'}{1+k'}\right)$ (downward)

(c) $E(k) = \dfrac{1+k}{2} E\left(\dfrac{2\sqrt{k}}{1+k}\right) + \dfrac{k'^2}{2} K(k)$ (upward)

(d) $E(k) = (1+k')E\left(\dfrac{1-k'}{1+k'}\right) - k'K(k)$ (downward).

Proof. Parts (*a*) and (*b*) are equivalent and follow from the previous discussion. We give a direct proof of (*b*) based on Ivory [1796]. This is also a third proof of Theorem 1.1. Let $l := (1-k')/(1+k')$. Then we have $\sqrt{l} = k/(1+k')$ and $1 + l^2 = 2(1+k'^2)/(1+k')^2$. Thus

$$\left(\frac{1+k'}{2}\right)K(k) = \frac{1}{2}\int_0^{\pi} \frac{d\theta}{\sqrt{(1+l^2) + 2l\cos 2\theta}}$$

on replacing $\sin^2\theta$ by $(1-\cos 2\theta)/2$. Then

$$\left(\frac{1+k'}{2}\right)K(k) = \frac{1}{2}\int_0^{\pi} (1+le^{-2i\theta})^{-1/2}(1+le^{2i\theta})^{-1/2}\, d\theta$$

$$= \frac{1}{2}\sum_{m,n=0}^{\infty} l^{m+n}\binom{-\frac{1}{2}}{m}\binom{-\frac{1}{2}}{n}\int_0^{\pi} e^{2i(m-n)\theta}\, d\theta .$$

Here we have used the binomial theorem twice. Since only the terms with $m = n$ are nonzero, we have

$$\left(\frac{1+k'}{2}\right)K(k) = \frac{\pi}{2}\sum_{n=0}^{\infty}\binom{-\frac{1}{2}}{n}^2 l^{2n} = \frac{\pi}{2} F\left(\frac{1}{2}, \frac{1}{2}; 1; l^2\right) = K(l)$$

on using (1.3.6). This completes (*b*). If $g(k) := 2\sqrt{k}/(1+k)$, then $g^{-1} = (1-k')/(1+k')$ and $[1+g'(k)]/2 = 1/(1+k)$. Now (*a*) follows by substituting $g(k)$ for k in (*b*). To derive part (*c*), we differentiate (*a*) to get, for $\dot{K} = dK/dk$,

(1.4.1) $$(1+k)\dot{K}(k) + K(k) = \dot{K}(g(k))\dot{g}(k) .$$

This is coupled with the differential equation (1.3.13) in the forms

(1.4.2) $$E(k) = kk'^2\dot{K}(k) + k'^2K(k)$$

and

(1.4.3) $$E(g(k)) = g(k)[g'(k)]^2\dot{K}(g(k)) + [g'(k)]^2K(g(k)) .$$

We now use (1.4.1) to eliminate $\dot{K}(g(k))$ from (1.4.3) and then employ (1.4.2) and (*a*) to solve for $E(g(k))$ in terms of $K(k)$ and $E(k)$. The algebraical details are left to the reader. Part (*d*) may be derived analogously from (*b*) or by substituting $g^{-1}(k)$ for k in (*c*). □

The transformations are termed upward and downward because, for $k \in (0,1)$, iterating (*a*) leads to a sequence of k values increasing to 1 and iterating (*b*) forms a sequence of k values decreasing to 0.

It is convenient to introduce homogeneous forms of E and K and to recast Theorem 1.2 in AGM terms.

Let

(1.4.4) $$I(a,b) := \int_0^{\pi/2} \frac{d\theta}{\sqrt{a^2\cos^2\theta + b^2\sin^2\theta}} = \frac{1}{a}K'\left(\frac{b}{a}\right)$$

(1.4.5) $$J(a,b) := \int_0^{\pi/2} \sqrt{a^2\cos^2\theta + b^2\sin^2\theta}\, d\theta = aE'\left(\frac{b}{a}\right).$$

Theorem 1.3

If $a_{n+1} := (a_n + b_n)/2$, $b_{n+1} := \sqrt{a_nb_n}$, and $0 < b_n < a_n$, then

(a) $I(a_{n+1}, b_{n+1}) = I(a_n, b_n)$

(b) $2J(a_{n+1}, b_{n+1}) - J(a_n, b_n) = a_nb_nI(a_n, b_n)$.

Proof. Part (*a*) has been observed in the second proof of the fundamental limit theorem (Theorem 1.1).

To see part (*b*), notice that if $k_n := c_n/a_n$, then $k'_n = b_n/a_n$,

$$2J(a_{n+1}, b_{n+1}) = 2a_{n+1}E\left(\sqrt{1 - \frac{b_{n+1}^2}{a_{n+1}^2}}\right) = 2a_{n+1}E(k_{n+1})$$

and

$$J(a_n, b_n) = a_nE\left(\sqrt{1 - \frac{b_n^2}{a_n^2}}\right) = a_nE(k_n) .$$

Recall that $c_n^2 = a_n^2 - b_n^2$. The relationship between k_{n+1} and k_n is given by

$$k_{n+1} = \frac{a_n - b_n}{a_n + b_n} = \frac{1 - k'_n}{1 + k'_n} .$$

Thus, establishing (b) is equivalent to establishing

$$2a_{n+1}E(k_{n+1}) - a_n E(k_n) = b_n K(k_n)$$

which on setting $a_{n+1} = (a_n + b_n)/2$ and dividing by a_n may be seen to be equivalent to part (d) of Theorem 1.2. □

These transformations may be iterated to produce quadratically convergent algorithms for K and E. (See also Exercise 1.)

Algorithm 1.1

(a) $$K'(k_0) = \frac{\pi}{2}\prod_{n=0}^{\infty}\frac{2}{1+k_n} = \frac{\pi}{2}\prod_{n=1}^{\infty}(1+k_n') \qquad \text{(upward iteration)}$$

where

$$k_{n+1} := \frac{2\sqrt{k_n}}{1+k_n} \quad \text{and} \quad k_0 \in (0, 1]\,.$$

(b) $$K(k_0) = \frac{\pi}{2}\prod_{n=0}^{\infty}\frac{2}{1+k_n'} = \frac{\pi}{2}\prod_{n=1}^{\infty}(1+k_n) \qquad \text{(downward iteration)}$$

where

$$k_{n+1} := \frac{1-k_n'}{1+k_n'} \quad \text{and} \quad k_0 \in [0, 1)\,.$$

The first product is the unique solution of Exercise 1a) analytic in a neighbourhood of 1 that takes the value $\pi/2$ at 1, while the second product is the unique solution of functional relation (b) of Theorem 1.2 that takes the value $\pi/2$ at 0 and is analytic in a neighbourhood of 0. This observation verifies that the above products are analytic in neighbourhoods of 0 and 1, respectively, since they are uniformly convergent products of analytic functions. Also, specifying the value of an analytic solution of either functional relation at any point in $(0, 1)$ in fact specifies the function at an infinite set of points with limit point within the domain of analyticity and hence uniquely defines the function up to a constant multiple of the value at the limit point. (See Exercise 4.)

The algorithms for E and K in AGM form are particularly attractive.

Algorithm 1.2

For $a_0 := 1$, $b_0 := k' \in (0, 1]$, and $c_0 := k$,

(a) $$K(k) = \frac{\pi}{2M(1, k')}$$

(b) $$E(k) = \left(1 - \sum_{n=0}^{\infty} 2^{n-1}c_n^2\right)K(k).$$

Proof. Part (a) is Theorem 1.1. For part (b) we use Theorem 1.3,

$$2J(a_{n+1}, b_{n+1}) - J(a_n, b_n) = a_n b_n I(a_n, b_n) = a_n b_n I(a_0, b_0)$$

and since $4a_{n+1}^2 - 2a_n^2 - 2a_n b_n = -c_n^2$,

$$2^{n+1}[J(a_{n+1}, b_{n+1}) - a_{n+1}^2 I(a_0, b_0)] - 2^n[J(a_n, b_n) - a_n^2 I(a_0, b_0)] = 2^{n-1}c_n^2 I(a_0, b_0)\,.$$

Thus on summing

(1.4.6) $$J(a_0, b_0) = \left(a_0^2 - \sum_{n=0}^{\infty} 2^{n-1}c_n^2\right)I(a_0, b_0)$$

which specializes to (b). Here we must observe that

$$\begin{aligned}\Delta_n &:= 2^n[a_n^2 I(a_n, b_n) - J(a_n, b_n)] \\ &= 2^n \int_0^{\pi/2} \frac{(a_n^2 - b_n^2)\sin^2\theta}{\sqrt{a_n^2\cos^2\theta + b_n^2\sin^2\theta}}\,d\theta \\ &= 2^n c_n^2 \int_0^{\pi/2} \frac{\sin^2\theta}{\sqrt{a_n^2\cos^2\theta + b_n^2\sin^2\theta}}\,d\theta\,.\end{aligned}$$

Thus $0 \le \Delta_n \le 2^n c_n^2 I(a_n, b_n)$, and Δ_n tends to zero as $n \to \infty$ since c_n^2 tends to zero quadratically. □

Comments and Exercises

The algorithms of the section provide remarkably efficient methods for the calculation of E and K and related functions. The analysis of these algorithms will be reserved for later chapters. We have restricted our attention in this section primarily to a real variable k. This is simplifying but entirely unnecessary. All of the algorithms and functional relations extend naturally to the complex domain. In fact, all the algorithms and functional equations of this section hold at least for $k \in \{\mathrm{re}(z) > 0\} - [1, \infty)$. The interested reader may readily establish the exact domains of validity for the various relations. The analysis of the AGM iteration for complex starting values is reasonably complicated. (See Cox [85].) The problem is to decide which root is appropriate in the computation of $b_{n+1} = \sqrt{a_n b_n}$. The right choice is made to ensure $|a_{n+1} - b_{n+1}| \le |a_{n+1} + b_{n+1}|$ [with im $(b_{n+1}/a_{n+1}) > 0$ in the case of equality]. The surprise is that no matter how the roots are chosen, the AGM iteration converges (provided $a_0 \ne -b_0$) though unless the right choice is made all but finitely often, the limit will be zero.

Exercise 5 on the Landen transform provides an algorithm for calculating incomplete elliptic integrals. We will revisit Landen's transform in Chapter 2. A wealth of formulae on the calculation of elliptic integrals may be found in King [24].

1. Show that

a) $K'(k) = \dfrac{2}{1+k} K'\left(\dfrac{2\sqrt{k}}{1+k}\right)$

b) $K'(k) = \dfrac{1}{1+k'} K'\left(\dfrac{1-k'}{1+k'}\right)$

c) $E'(k) = (1+k)E'\left(\dfrac{2\sqrt{k}}{1+k}\right) - kK'(k)$

d) $E'(k) = \left(\dfrac{1+k'}{2}\right)E'\left(\dfrac{1-k'}{1+k'}\right) + \dfrac{k^2}{2} K'(k)$

and observe that K'/K satisfies a multiplication theorem, namely,

e) $\dfrac{K'}{K}(k) = 2\dfrac{K'}{K}\left(\dfrac{2\sqrt{k}}{1+k}\right) = \dfrac{1}{2}\dfrac{K'}{K}\left(\dfrac{1-k'}{1+k'}\right)$.

Show that for every integer n there is a unique algebraic $x \in (0,1)$ so that

f) $\dfrac{K'}{K}(x) = 2^n$.

2. Show that if $k_{n+1} := (1-k_n')/(1+k_n')$ and $j_n := \sqrt{k_{2n}}$, then

a) $j_{n+1} = \dfrac{1 - \sqrt[4]{1-j_n^4}}{1 + \sqrt[4]{1-j_n^4}}$

and hence

b) $K(x) = \dfrac{4}{(1+\sqrt{x'})^2} K\left(\left[\dfrac{1-\sqrt[4]{1-x^4}}{1+\sqrt[4]{1-x^4}}\right]^2\right)$.

Also

c) $K(j_0^2) = \dfrac{\pi}{2}\prod_{n=0}^{\infty} \dfrac{4}{(1+\sqrt[4]{1-j_n^4})^2} = \dfrac{\pi}{2}\prod_{n=1}^{\infty}(1+j_n)^2$.

Show that j_n converges quartically to zero.

3. (*The quartic AGM*) Let a_n, b_n, and c_n satisfy the AGM relations. Set $\alpha_n := a_{2n}^{1/2}$ and $\beta_n := b_{2n}^{1/2}$. Show that

a) $\alpha_{n+1} = \dfrac{\alpha_n + \beta_n}{2}$

and

b) $\beta_{n+1} = \left(\dfrac{\alpha_n^3\beta_n + \beta_n^3\alpha_n}{2}\right)^{1/4}$.

Show also that

c) $\sum_{n=0}^{\infty} 2^{n-1}c_n^2 = \sum_{n=0}^{\infty} 4^n\left[\alpha_n^4 - \left(\dfrac{\alpha_n^2+\beta_n^2}{2}\right)^2\right]$.

Show that the convergence is governed by

d) $\alpha_{n+1}^4 - \beta_{n+1}^4 = \dfrac{(\alpha_n - \beta_n)^4}{16}$.

Derive the following quartic algorithms. For $\alpha_0 := 1$ and $\beta_0 := \sqrt{k'} \in (0,1]$,

e) $K(k) = \dfrac{\pi}{2 \lim \alpha_n^2}$.

f) $\dfrac{E(k)}{K(k)} = 1 - \sum_{n=0}^{\infty} 4^n\left[\alpha_n^4 - \left(\dfrac{\alpha_n^2+\beta_n^2}{2}\right)^2\right]$.

4. Consider a functional relation

$$F(z) = s(z)F(g(z)) \qquad F(0) = \alpha$$

where s and g are analytic in some complex neighbourhood U of zero. Suppose that, for some $p > 1$, $\lim_{n\to\infty} g^{(n)}(z) \to 0$ with pth order convergence uniformly on U. [$g^{(n)}$ denotes g composed with itself n times.] Show that the above relation has a unique nonzero analytic solution on U if and only if $s(0) = 1$.

5. (*The Landen transform*) Consider the incomplete elliptic integral of the first kind

$$F(\phi, k) := \int_0^{\phi} \frac{d\theta}{\sqrt{1 - k^2\sin^2\theta}} \qquad k \in [0,1), \quad \phi \ge 0.$$

Show, as in the second proof of Theorem 1.1, that if we set $k_{n+1} := (1-k'_n)/(1+k'_n)$ and $\tan(\phi_{n+1}-\phi_n) = k'_n \tan\phi_n$, then

a) $F(\phi_{n+1}, k_{n+1}) = (1+k'_n)F(\phi_n, k_n) \qquad k_{n+1} \le k_n\,, \quad \phi_{n+1} \ge \phi_n$

and

b) $F(\phi_0, k_0) = \left(\prod_{n=0}^{\infty} \frac{2}{1+k'_n}\right) \lim_{n\to\infty} \left(\frac{\phi_n}{2^n}\right).$

Show that if $k_{n+1} := 2\sqrt{k_n}/(1+k_n)$ and $\sin(2\phi_{n+1}-\phi_n) := k_n \sin\phi_n$, then

c) $F(\phi_{n+1}, k_{n+1}) = \frac{1}{2}(1+k_n)F(\phi_n, k_n) \qquad k_{n+1} \ge k_n\,, \quad \phi_{n+1} \le \phi_n$

and

d) $F(\phi_0, k_0) = \left(\prod_{n=0}^{\infty} \frac{2}{1+k_n}\right) \log\tan\left(\frac{\pi}{4} + \frac{1}{2}\lim_{n\to\infty} \phi_n\right).$

e) Establish the quadratic convergence.

Similar methods for calculating incomplete second and third integrals may be found in King [24]. (See also Section 2.7.)

6. Prove Euler's addition theorem. Let $g(x) := (1-x^2)(1-k^2x^2)$. Then

$$\int_0^a \frac{dx}{\sqrt{g(x)}} + \int_0^b \frac{dx}{\sqrt{g(x)}} = \int_0^c \frac{dx}{\sqrt{g(x)}}$$

where $c := [b\sqrt{g(a)} + a\sqrt{g(b)}]/\sqrt{1-k^2a^2b^2}$. This result, which dates from 1753, is, according to Birkhoff [73], the "first notable theorem about elliptic integrals."

1.5 *JACOBI'S DIFFERENTIAL EQUATION AND A FOURTH PROOF OF THE FUNDAMENTAL LIMIT THEOREM*

The second-order linear differential equation (1.3.8) satisfied by K and K' is

$$(k^3-k)\frac{d^2y}{dk^2} + (3k^2-1)\frac{dy}{dk} + ky = 0\,.$$

Equivalently

$$G(k) := k^{1/2}k'K(k) \qquad \text{and} \qquad G^*(k) := k^{1/2}k'K'(k)$$

satisfy

$$\frac{d^2y}{dk^2} = -\frac{1}{4k^2}\left(\frac{1+k^2}{1-k^2}\right)^2 y\,. \tag{1.5.1}$$

Also, the functional relations [(Theorem 1.2(*a*) and Exercise 1a) of Section 1.4] become

$$G(k) := \frac{1+k}{\sqrt{2}}\sqrt{\frac{k^{1/2}}{1-k}}\; G\left(\frac{2\sqrt{k}}{1+k}\right) \tag{1.5.2}$$

and

$$G^*(k) := \sqrt{2}(1+k)\sqrt{\frac{k^{1/2}}{1-k}}\; G^*\left(\frac{2\sqrt{k}}{1+k}\right). \tag{1.5.3}$$

If we set $g(k) := 2\sqrt{k}/(1+k)$, these become

$$G(k) = \sqrt{\frac{1}{2\dot g(k)}}\; G(g(k)) \tag{1.5.4}$$

and

$$G^*(k) = \sqrt{\frac{2}{\dot g(k)}}\; G^*(g(k))\,. \tag{1.5.5}$$

Theorem 1.4

Suppose that f, $\dot g$, and α are all in $C^2(0,1)$ and that g maps $[0,1]$ into $[0,1]$. If, for $x \in (0,1)$,

(*a*) $\dfrac{d^2f(x)}{dx^2} = \alpha(x)f(x)$

and

(*b*) $f(x) = \sqrt{\dfrac{c}{\dot g(x)}}\; f(g(x)) \qquad c$ a constant

then

(*c*) $\alpha(x) = (\dot g(x))^2\alpha(g(x)) - \dfrac{1}{2}\left[\dfrac{\dddot g(x)}{\dot g(x)} - \dfrac{3}{2}\left(\dfrac{\ddot g(x)}{\dot g(x)}\right)^2\right].$

Proof. Use (*b*) to change variables in (*a*). Then, on suppressing x,

$$\alpha f = \ddot f = (2\dot p\dot g + p\ddot g)\frac{df(g)}{dg} + \ddot p f(g) + \dot g^2 p\,\frac{d^2f(g)}{dg^2} \tag{1.5.6}$$

where $p := \sqrt{c/\dot g}$ (remember that $\dot\alpha$ is the derivative with respect to x). Also, from (*a*) and (*b*),

$$\ddot f = \alpha f = \alpha p f(g)\,. \tag{1.5.7}$$

Substituting (1.5.7) into (1.5.6) to eliminate $\ddot f$ yields

$$(1.5.8) \qquad \frac{d^2f(g)}{dg^2} = -\frac{2\dot{p}\dot{g}+p\ddot{g}}{\dot{g}^2p}\frac{df(g)}{dg} + \left(\frac{\alpha p - \ddot{p}}{\dot{g}^2p}\right)f(g)$$

which on comparison with (a) gives

$$\frac{\alpha p - \ddot{p}}{\dot{g}^2p} = \alpha(g)$$

since $2\dot{p}\dot{g}+p\ddot{g}=0$. Finally we compute p, $\dot{p}$ and $\ddot{p}$ in terms of g to get (c). □

The bracketed quantity on the right of (c) is often called the *Schwartz derivative* of g.

Corollary 1.1 **(*Jacobi's Differential Equation*)**

Suppose $G(x) := x^{1/2}x'K(x)$. If p and g are algebraic functions that map $[0,1]$ into $[0,1]$ and

$$G(x) = p(x)G(g(x))$$

then g satisfies an algebraic differential equation

$$r(x) = [\dot{g}(x)]^2r(g(x)) - \frac{1}{2}\left[\frac{\dddot{g}(x)}{\dot{g}(x)} - \frac{3}{2}\left(\frac{\ddot{g}(x)}{\dot{g}(x)}\right)^2\right]$$

where

$$r(x) := -\frac{1}{4x^2}\left(\frac{1+x^2}{1-x^2}\right)^2.$$

Proof. We may assume that $G(x)$ does not satisfy any equation of the form

$$\dot{G}(x) = \beta(x)G(x)$$

with β algebraic since by (1.3.13), (1.3.10), and (1.3.11) $\dot{G}/G$ has a logarithmic singularity at 1. Thus since G satisfies equation (1.5.1), as in (1.5.6) we must have

$$2\dot{p}\dot{g} + p\ddot{g} = 0$$

or

$$p = \sqrt{\frac{c}{\dot{g}}}.$$

The result now follows from Theorem 1.4 applied to (1.5.1). □

This corollary has a converse which provides an algorithmic check on whether g is an algebraic transform of K. (See Exercise 1.) Theorem 1.4 has a partial converse.

Theorem 1.5

Suppose that f, $\dot{g}$, and α are all in $C^2(0,1)$ and that g maps $[0,1]$ into $[0,1]$. Suppose that

$$(a) \quad \alpha(x) = (\dot{g}(x))^2\alpha(g(x)) - \frac{1}{2}\left[\frac{\dddot{g}(x)}{\dot{g}(x)} - \frac{3}{2}\left(\frac{\ddot{g}(x)}{\dot{g}(x)}\right)^2\right]$$

and

$$(b) \quad \frac{d^2f(x)}{dx^2} = \alpha(x)f(x).$$

Then

$$(c) \quad \sqrt{\frac{c}{\dot{g}}}\, f(g(x))$$

is also a solution of (b).

Proof. This is essentially the computation of (1.5.8). Replacing f by $\sqrt{c/\dot{g}}\, f(g)$ leaves (b) invariant provided (a) holds. □

We now offer a proof of Theorem 1.1 based on Theorem 1.5.

Fourth proof of the fundamental limit theorem. For

$$\alpha(x) := -\frac{1}{4x^2}\left(\frac{1+x^2}{1-x^2}\right)^2 \quad \text{and} \quad g(x) := \frac{2\sqrt{x}}{1+x}$$

condition (a) of Theorem 1.5 holds. This is a tedious though (eventually) entirely rational calculation. Thus if G is a solution of

$$\frac{d^2G(x)}{dx^2} = \alpha(x)G(x)$$

then so is

$$\sqrt{\frac{1}{2\dot{g}(x)}}\, G(g(x)).$$

However, the above second-order linear differential equation has a regular singular point at zero and has fundamental solutions of the form

$$\sqrt{x}g_1(x)$$

and

$$\sqrt{x}g_1(x)\log x + \sqrt{x}g_2(x)$$

where g_1 and g_2 are analytic and nonzero. Now observe that

$$\frac{G(x)}{\sqrt{x}} = x'K(x)$$

is analytic and nonzero in a neighbourhood of zero, and hence $G(x)$ must be a constant multiple of the first fundamental solution. Moreover,

$$\frac{1}{\sqrt{x}}\sqrt{\frac{1}{2\dot{g}(x)}}\,G(g(x))$$

cannot have a logarithmic singularity at zero, and hence $(2\dot{g}(x))^{-1/2}G(g(x))$ must also be a constant multiple of the first fundamental solution. In particular for some c,

$$G(x) = c\sqrt{\frac{1}{2\dot{g}(x)}}\,G(g(x))\,.$$

If we multiply by $\sqrt{g(x)/x}$ and take the limit as $x \to 0$, we deduce that $c = 1$. We have thus proven that G satisfies equation (1.5.4). Equation (1.5.4) transforms into

$$K(x) = \frac{1}{1+x}K(g(x))$$

and we have shown that K, defined as an analytic solution of the differential equation (1.3.8), satisfies the above functional relation, and hence we have found an analytic invariant for the Legendre form of the AGM. [See (1.1.10).] □

Comments and Exercises

A form of Jacobi's highly nonlinear differential equation may be found in Cayley [1895], which is an excellent account of nineteenth-century elliptic function theory with particular emphasis on the transformation theory.

The general question of when a functional relation

$$f(x) = p(x)f(g(x))$$

has a closed-form solution in terms of familiar functions is difficult. We shall consider it again later. Theorems 1.4 and 1.5 do, however, suggest how one

might proceed to check whether a solution of the above functional relation satisfies a second-order differential equation with rational coefficients. (See Exercises 2 and 3.)

1. Suppose that $g(x)$ is an algebraic function, g maps $[0, 1]$ into $[0, 1]$, and $g(0) = 0$. Suppose that g satisfies the algebraic differential equation of Corollary 1.1. Show, as the fourth proof of Theorem 1.1, that there exists a constant c so that

$$G(x) = \sqrt{\frac{c}{\dot{g}(x)}}\,G(g(x))\,.$$

2. Suppose that

$$F(x) = \sqrt{\frac{1}{2\dot{g}(x)}}\,F(g(x))$$

and that

$$\frac{d^2F(x)}{dx^2} = r(x)F(x)$$

where $F(x)/\sqrt{x}$ is analytic in a neighbourhood of zero, r is a rational function, and $g(x) := 2\sqrt{x}/(1+x)$. Without identifying F explicitly, show that r has double poles at 0 and 1. (Considerations of this nature can turn the fourth proof into less of a verification.)

3. Suppose that α, p, and g mapping $[0, 1]$ into $[0, 1]$ are algebraic, that

$$\frac{d^3f(x)}{dx^3} = \alpha(x)f(x) \qquad x \in (0, 1)$$

and that

$$f(x) = p(x)f(g(x)) \qquad x \in (0, 1)\,.$$

Suppose also that f does not satisfy a linear differential equation with algebraic coefficients of order less than 3. Show that

$$g(x) = \frac{ax+b}{cx+d} \qquad \text{and} \qquad p(x) = e(cx+d)^2\,.$$

1.6 *LEGENDRE'S RELATION*

The four quantities K, E, K', and E' are related by a remarkable relation.

Theorem 1.6 (Legendre's Relation)

For $0<k<1$,

$$E(k)K'(k)+E'(k)K(k)-K(k)K'(k)=\frac{\pi}{2}.$$

Proof. Let $G:=k^{1/2}k'K$ and $G^*:=k^{1/2}k'K'$, as in Section 1.5. Then, by (1.5.1),

$$\frac{\ddot{G}}{G}=\frac{\ddot{G}^*}{G^*}$$

and hence there is a constant c so that

$$\dot{G}G^*-\dot{G}^*G=c. \tag{1.6.1}$$

In other words, the Wronskian of G and G^* is constant. On writing G and G^* in terms of K and K' this becomes

$$k(1-k^2)(\dot{K}K'-K\dot{K}')=c. \tag{1.6.2}$$

We now use equation (1.3.13),

$$\frac{dK}{dk}=\frac{E-(1-k^2)K}{k(1-k^2)}$$

to eliminate the derivatives in (1.6.2) and deduce that

$$EK'+E'K-KK'=c. \tag{1.6.3}$$

It remains to evaluate the constant c. This may be done directly from the series expansion at zero (see Section 1.3, Exercise 5), or by using Exercise 4 of Section 1.3. □

We define the *gamma* and *beta* functions by

$$\Gamma(x):=\int_0^\infty e^{-t}t^{x-1}\,dt \qquad \mathrm{re}(x)>0 \tag{1.6.4}$$

$$\beta(x,y):=\int_0^1 t^{x-1}(1-t)^{y-1}\,dt \qquad \mathrm{re}(x),\ \mathrm{re}(y)>0. \tag{1.6.5}$$

The function Γ satisfies the functional relation

$$\Gamma(x)\Gamma(1-x)=\frac{\pi}{\sin\pi x}. \tag{1.6.6}$$

The relationship between Γ and β is

$$\beta(x,y)=\frac{\Gamma(x)\Gamma(y)}{\Gamma(x+y)}. \tag{1.6.7}$$

These standard results will be discussed further in Section 3.6. Our present objective is to evaluate $K(1/\sqrt{2})$ and $E(1/\sqrt{2})$.

Theorem 1.7

$$K\left(\frac{1}{\sqrt{2}}\right)=\frac{\Gamma^2(\frac14)}{4\sqrt{\pi}}$$

and

$$E\left(\frac{1}{\sqrt{2}}\right)=\frac{4\Gamma^2(\frac34)+\Gamma^2(\frac14)}{8\sqrt{\pi}}.$$

Proof.

$$K\left(\frac{1}{\sqrt{2}}\right)=\int_0^1\frac{dt}{\sqrt{(1-t^2)(1-\frac12 t^2)}}=\sqrt{2}\int_0^1\frac{dt}{\sqrt{(1-t^2)(2-t^2)}}.$$

The change of variables $x^2:=t^2/(2-t^2)$ gives

$$K\left(\frac{1}{\sqrt{2}}\right)=\sqrt{2}\int_0^1\frac{dt}{\sqrt{1-t^4}}.$$

The above arclemniscate (giving the arclength of a lemniscate) can be evaluated in terms of β. We set $u:=t^4$ and see that

$$K\left(\frac{1}{\sqrt{2}}\right)=\frac{\sqrt{2}}{4}\int_0^1 u^{1/4-1}(1-u)^{1/2-1}\,dt$$
$$=\frac{\sqrt{2}}{4}\,\beta\left(\frac14,\frac12\right)=\frac{\sqrt{2}}{4}\,\frac{\Gamma(\frac14)\Gamma(\frac12)}{\Gamma(\frac34)}.$$

Finally, by (1.6.6),

$$\Gamma\left(\frac12\right)=\sqrt{\pi} \quad\text{and}\quad \Gamma\left(\frac34\right)=\frac{\sqrt{2}\pi}{\Gamma(\frac14)}.$$

The evaluation of $E(1/\sqrt{2})$ is left as Exercise 3. □

Since $K(1/\sqrt{2}) = K'(1/\sqrt{2})$ and $E(1/\sqrt{2}) = E'(1/\sqrt{2})$, the evaluation of $K(1/\sqrt{2})$ and $E(1/\sqrt{2})$ gives an alternate route to evaluating the constant in Legendre's identity that avoids developing the asymptotic expansion of K' at zero.

Comments and Exercises

We observe that at $1/\sqrt{2}$ Legendre's identity reduces to

$$K\left(\frac{1}{\sqrt{2}}\right)\left[2E\left(\frac{1}{\sqrt{2}}\right) - K\left(\frac{1}{\sqrt{2}}\right)\right] = \frac{\pi}{2}$$

or

$$\frac{2K(1/\sqrt{2})}{\pi}\left[\frac{2E(1/\sqrt{2})}{\pi} - \frac{K(1/\sqrt{2})}{\pi}\right] = \frac{1}{\pi}.$$

Now K/π and E/π can be calculated quadratically by Algorithm 1.2 using only the operations of addition, multiplication, division, and square-root extraction and commencing with a rational starting value. This provides an excellent approach to calculating π—an approach we will pursue in some detail in Chapters 2 and 5.

Legendre derives the constant in (1.6.3) by evaluating $K((\sqrt{3} \pm 1)/\sqrt{8})$. (See Whittaker and Watson [27] and Exercise 6.) Note that $(\sqrt{3}-1)/\sqrt{8}$ and $(\sqrt{3}+1)/\sqrt{8}$ are complementary. It transpires that

$$\frac{K'}{K}\left(\frac{\sqrt{3}-1}{\sqrt{8}}\right) = \sqrt{3}.$$

Values of k for which K'/K is a rational surd are of considerable interest and importance. (See Chapter 4.) Such k are called *singular values*, the simplest of which is $1/\sqrt{2}$, where

$$\frac{K'}{K}\left(\frac{1}{\sqrt{2}}\right) = 1.$$

1. Show that

$$E\left(\frac{1}{\sqrt{2}}\right) = \frac{4\Gamma^2(\frac{3}{4}) + \Gamma^2(\frac{1}{4})}{8\sqrt{\pi}}.$$

Start by writing

$$E\left(\frac{1}{\sqrt{2}}\right) = \int_0^1 \frac{\sqrt{1-\frac{1}{2}t^2}}{\sqrt{1-t^2}}\,dt.$$

Then set $u := \sqrt{1-t^2}$ and show that

$$E\left(\frac{1}{\sqrt{2}}\right) = \frac{1}{\sqrt{2}}\int_0^1 \frac{u^2}{\sqrt{1-u^4}}\,du + \frac{1}{\sqrt{2}}\int_0^1 \frac{1}{\sqrt{1-u^4}}\,du.$$

2. Show that

$$K\left(\frac{1}{\sqrt{2}}\right)\dot{K}\left(\frac{1}{\sqrt{2}}\right) = \frac{\pi}{\sqrt{2}}.$$

3. Show that

a) $$\int_0^\infty e^{-t^2}\,dt = \frac{\sqrt{\pi}}{2}.$$

Show first that

$$f(x) := \left(\int_0^x e^{-t^2}\,dt\right)^2 \quad \text{and} \quad g(x) := \int_0^1 \frac{e^{-x^2(t^2+1)}}{t^2+1}\,dt$$

satisfy $f' + g' = 0$ and $f + g = \pi/4$.

b) Use a) to show that $\Gamma(\frac{1}{2}) = \sqrt{\pi}$.

4. Use Theorem 1.2 to deduce that

$$\frac{K'}{K}(\sqrt{2}-1) = \sqrt{2}.$$

[In fact $K(\sqrt{2}-1) = (\sqrt{2}+1)^{1/2}\Gamma(\frac{1}{8})\Gamma(\frac{3}{8})/2^{13/4}\pi^{1/2}$.] Thus $\sqrt{2}-1$ is a second singular value. We return to both singular values and Γ function evaluations of K subsequently.

5. Establish Legendre's relation directly from (1.3.12) and (1.3.13) applied to E, E', K, and K'. Use Exercise 4 of Section 1.3 to determine the constant.

6. From the general theory of the Weierstrass function developed in the next section, or more directly, one can show (Whittaker and Watson [27, p. 516]) that for $a, b > 0$,

$$\int_{-a}^{a} \frac{dx}{\sqrt{(a^2-x^2)(b^2+x^2)}} = \int_e^\infty \frac{dt}{\sqrt{4t^3 - g_2 t - g_3}}$$

where e is the real root of the above cubic and

$$g_2 := \tfrac{1}{12}(a^2-b^2)^2 - (ab)^2$$

$$g_3 := -\tfrac{1}{216}(a^2-b^2)[(a^2-b^2)^2 + 36(ab)^2].$$

a) If $g_2 = 0$, then

$$a^2 + b^2 = 2\sqrt{3}|2g_3|^{1/3} \qquad a^2 - b^2 = -3(2g_3)^{1/3}.$$

b) If $g_2 = 0$ and $g_3 > 0$, then

i) $$\int_e^\infty \frac{dt}{\sqrt{4t^3 - g_3}} = \frac{2}{\sqrt{a^2+b^2}} K\left(\frac{a}{\sqrt{a^2+b^2}}\right)$$

ii) $$\int_{-e}^\infty \frac{dt}{\sqrt{4t^3 + g_3}} = \frac{2}{\sqrt{a^2+b^2}} K\left(\frac{b}{\sqrt{a^2+b^2}}\right).$$

c) Let $e := g_3 := \frac{1}{2}$. Then $a^2 + b^2 = 2\sqrt{3}$, and bi) gives

$$2\times 3^{-1/4}K = \int_1^\infty \frac{dt}{\sqrt{t^3-1}} = \frac{1}{3}\,\beta\left(\frac{1}{6}, \frac{1}{2}\right).$$

Also, bii) gives

$$2\times 3^{-1/4}K' = \int_{-1}^\infty \frac{dt}{\sqrt{t^3+1}} = \int_0^1 \frac{dt}{\sqrt{1-t^3}} + \int_0^\infty \frac{dt}{\sqrt{1+t^3}}\,.$$

Now substitution of $s := 1/t$ and $s := (1+t^3)^{-1/2}$, respectively, leads to

$$2\times 3^{-1/4}K' = \frac{1}{3}\left[\beta\left(\frac{1}{3}, \frac{1}{2}\right) + \beta\left(\frac{1}{6}, \frac{1}{3}\right)\right] = \frac{1}{\sqrt{3}}\,\beta\left(\frac{1}{6}, \frac{1}{2}\right).$$

d) Thus when $k := \sin(\pi/12) = (\sqrt{3}-1)/2\sqrt{2}$

$$K'(k) = \sqrt{3}K(k)$$

and

$$K\left(\frac{\sqrt{3}-1}{2\sqrt{2}}\right) = 3^{-1/4}\,\frac{\Gamma(\frac{1}{6})\Gamma(\frac{1}{3})}{4\sqrt{\pi}} = \frac{3^{1/4}\Gamma(\frac{1}{3})^3}{2^{7/3}\pi}\,.$$

This evaluates K in terms of Γ functions and shows that $\sin(\pi/12)$ is a third singular value.

1.7 *ELLIPTIC FUNCTIONS*

The study of elliptic functions began in the 1820s when Abel and Jacobi independently discovered that the inverses of elliptic integrals are doubly periodic functions. As noted earlier, they had been anticipated by Gauss who at the turn of the century had studied a particular elliptic function, the lemniscate sine. This work, however, had not been published. This was one of the critical discoveries of the era and was vital to the concomitant development of complex analysis and the later development of modular and automorphic functions.

Except for minimal application in Sections 2.6 and 2.7, we have no great need for this body of material and offer only a brief sketch of this attractive theory, primarily in the exercises at the end of this section. Details may be found in Whittaker and Watson [27] and, more recently, in Bowman [53], Du Val [73], Eagle [58], and Lang [73].

An *elliptic function* is a meromorphic function with two periods w_1 and w_2, with $\operatorname{im}(w_1/w_2) \neq 0$. That is, for all z, $f(z) = f(z+w_1) = f(z+w_2)$. We assume that w_1 and w_2 are minimal in the sense that they are not multiples of any smaller period. The function f is completely determined by its behaviour on any parallelogram that is a translate of the parallelogram with vertices 0, w_1, w_2, and $w_1 + w_2$. Any such parallelogram is called *fundamental*. Associated with the periods w_1 and w_2 there is the lattice $L := \{nw_1 + mw_2 | m, n \text{ integers}\}$. It transpires that given any lattice L there exist elliptic functions with the appropriate associated periods. However, there are not many such functions. As we shall indicate in the exercises, any two such functions are connected by an algebraic equation. The circular functions may be thought of as degenerate elliptic functions (one of the periods is infinite), as may rational functions (both periods infinite).

A function f is said to have an *algebraic addition theorem* if there exists a polynomial Ω in three variables with complex coefficients so that for $x, y \in \mathbb{C}$,

$$\Omega(f(x), f(y), f(x+y)) = 0\,.$$

One of the many remarkable facts, due in part to Weierstrass, is that a meromorphic function has an algebraic addition theorem if and only if it is elliptic or degenerate elliptic. (See Exercises 11, 12 and 13 or Hancock [09].)

The Jacobian elliptic function sn is defined by

$$u = \int_0^{\operatorname{sn}(u,k)} \frac{dt}{\sqrt{(1-t^2)(1-k^2t^2)}}\,. \tag{1.7.1}$$

The value k is thought of as a parameter and is often omitted. It is true, though not obvious, that $\operatorname{sn}(u)$ is a meromorphic function with periods $4K$ and $2iK'$ and, hence, is elliptic. (See Exercise 2 of Section 2.7.) The two other basic Jacobian elliptic functions are cn and dn, defined by

$$u = \int_1^{\operatorname{cn}(u,k)} \frac{dt}{\sqrt{(1-t^2)(k'^2+k^2t^2)}} \tag{1.7.2}$$

and

$$u = \int_1^{\operatorname{dn}(u,k)} \frac{dt}{\sqrt{(1-t^2)(t^2-k'^2)}}\,. \tag{1.7.3}$$

Note that sin and tanh are limiting cases

$$\mathrm{sn}(u, 0) = \sin u$$

and

$$\mathrm{sn}(u, 1) = \tanh u\,.$$

A "half-angle" formula for sn is

$$\mathrm{sn}^2\left(\frac{u}{2}\right) = \frac{1 - \sqrt{1 - \mathrm{sn}^2(u)}}{1 + \sqrt{1 - k^2\,\mathrm{sn}^2(u)}}\,. \tag{1.7.4}$$

Again this is not obvious. It is worth observing that a half-angle formula is a specialization ($x = y$) of an algebraic addition theorem. These matters are pursued further in Sections 2.6 and 2.7. In particular, Exercise 6 of Section 2.7 presents an addition formula for sn.

Comments and Exercises

The following exercises develop some of the elementary theory of elliptic functions. The approach is via the Weierstrass p function and is standard. See, for example, Erdélyi et al. [53], Du Val [73], or Lang [73].

1. Show that the elliptic functions (with respect to a fixed lattice L) form a field that is closed under differentiation.
2. Show that an entire elliptic function is constant.
3. Let f be elliptic with respect to L. Assume f is nonconstant. Let P be a fundamental parallelogram whose boundary B contains no zeros or poles of f.
   a) Show that the sum of the residues of f in P is 0 by using the periodicity of f to show that $\int_B f = 0$. Thus any nontrivial elliptic function has at least two poles in P. The number of poles in P, counted according to multiplicity, is called the *order* of f.
   b) Show that f has the same number of zeros as poles in P counted according to multiplicity. *Hint*: Consider $\int_B \dot{f}/f$ and observe that $\dot{f}/f$ is elliptic.
   c) Show that f assumes every complex value exactly order of f times in P.
4. Show that the Weierstrass function

$$p(z) := \frac{1}{z^2} + \sum_{w \in L'} \left[\frac{1}{(z-w)^2} - \frac{1}{w^2}\right]$$

   is meromorphic, even, and has double poles at each lattice point $[L' := L - (0, 0)]$.
5. a) Show that

$$\dot{p}(z) = -2 \sum_{w \in L} \frac{1}{(z-w)^3}\,.$$

   Show that $\dot{p}$ is an odd elliptic function of order 3.
   b) Use a) and the fact that p is even to deduce that p is elliptic. Observe that p has order 2.
6. Show that every even elliptic function f is a rational function of p. *Hint*: Observe that if z is a zero of f in P (a fundamental parallelogram) then so is $-z \bmod L$. (By $-z \bmod L$ we mean the unique point in P, that is equivalent to $-z$ with respect to L; that is, there exist m and n so that $mw_1 + nw_2 - z = -z \bmod L$ and $-z \bmod L \in P$.) Observe that there are exactly four points in P where $z = -z \bmod L$ $(0, w_1/2, w_2/2, (w_1 + w_2)/2)$ and that if f has a zero at one of these four points, it must have even multiplicity. Consider

$$g(z) := \Pi\,[p(z) - p(z_i)]^{\delta_i}$$

   where the product is extended over the zeros of f, choosing only one representative from each pair $(z, -z \bmod L)$ and where δ_i is the multiplicity of the zero (except in the case $z_i = -z_i \bmod L$, in which case δ_i is half the multiplicity). Now show that f and g have the same zeros with the same multiplicities. Treat the poles similarly.
7. Show that any elliptic function f is a rational function of p and $\dot{p}$. *Hint*: Consider

$$f(z) = \frac{f(z) + f(-z)}{2} + \frac{([f(z) - f(-z)]/2)\dot{p}(z)}{\dot{p}(z)}$$

   which decomposes f into an even elliptic function and an even elliptic function divided by $\dot{p}$.
8. Show that there exist constants g_2 and g_3 so that

$$[\dot{p}(z)]^2 = 4p^3(z) - g_2 p(z) - g_3\,.$$

   Hint: Consider the order of the pole of $\dot{p}^2 - 4p^3$ at zero. Observe that g_2 and g_3 depend on L. Different lattices lead to uniformizations (parametrizations) of different cubics.
9. Show that any two nonconstant elliptic functions f and g (with respect to the same lattice) satisfy an algebraic equation

$$\Omega(f, g) = 0$$

   where Ω is a polynomial in two variables with complex coefficients.
10. Suppose that f is meromorphic and singly periodic with period w.

Suppose that f assumes no value infinitely many times in any period strip. Show that f is a rational function of $e^{2\pi iz/w}$. (One can use this as a definition of the class of trigonometric or circular functions.)

11. Prove that the function p satisfies the algebraic addition theorem

$$p(x+y)=\frac{1}{4}\left[\frac{\dot{p}(x)-\dot{p}(y)}{p(x)-p(y)}\right]^2-p(x)-p(y)\,.$$

Hint: Show that, as a function of x,

$$\frac{1}{4}\left[\frac{\dot{p}(x)-\dot{p}(y)}{p(x)-p(y)}\right]^2-p(x)-p(x+y)$$

has no singularities at the points 0, $\pm y$ and, hence, is independent of x. With Exercise 8, this is an addition theorem.

12. Show that every elliptic function f has an algebraic addition theorem. *Hint*: Connect f to p algebraically and use the addition theorem for p.

13. Show that if f meromorphic and has an algebraic addition theorem Ω, then either

a) f is a rational function,
b) f is a trigonometric function, or
c) f is an elliptic function.

Hint: Case a) occurs if f has a pole at infinity. So suppose to the contrary that infinity is an essential singularity. Now for some w, $f(z)=w$ has infinitely many solutions $z_1, z_2, \ldots$. Choose z^* so that $z^*, z^*+z_1, z^*+z_2, \ldots$ are not poles of f. Show that there exist m and n, both less than a constant depending only on Ω, so that $f(z^*+z_n)=f(z^*+z_m)$. Show that in any neighbourhood there exist infinitely many points and some n and m so that $f(z+z_n)=f(z+z_m)$. Thus f has a period z_n-z_m. Case b) occurs if f has only one period, in which case f can assume any value only finitely many times within any period strip. In that case Exercise 10 applies. Otherwise we have case c).

Chapter Two

Theta Functions and the Arithmetic-Geometric Mean Iteration

Abstract. *In this chapter we solve the AGM iteration in theta function terms and derive a variety of useful properties of theta functions. The central tool is the Poisson summation formula. These results are then applied to produce quadratically convergent products for π and e^π and quadratically convergent sums for π.*

We finish the chapter by discussing the Landen transform and the relationship between theta and elliptic functions.

2.1 *A THETA SERIES SOLUTION TO THE AGM*

The basic *theta functions* are defined for $|q|<1$ by

(2.1.1) $$\theta_2(q):=\sum_{n=-\infty}^{\infty} q^{(n+1/2)^2} \qquad \theta_2(0)=0\,.$$

(2.1.2) $$\theta_3(q):=\sum_{n=-\infty}^{\infty} q^{n^2} \qquad \theta_3(0)=1\,.$$

(2.1.3) $$\theta_4(q):=\sum_{n=-\infty}^{\infty} (-1)^n q^{n^2} \qquad \theta_4(0)=1\,.$$

These series are more properly viewed as functions of two complex variables one of which is presently set to zero. (See Section 2.6.) Theta functions have various number theoretic connections. Note that θ_3 is a generating function for squares, while as $\theta_4(q)=\theta_3(-q)$, θ_4 also considers the parity of the square. Thus

$$\theta_3(q)+\theta_4(q)=2\sum_{n \text{ even}} q^{n^2}=2\theta_3(q^4)\,. \tag{2.1.4}$$

Also

$$\theta_3^2(q)=\sum_{n=0}^{\infty} r_2(n)q^n \qquad \theta_4^2(q)=\sum_{n=0}^{\infty}(-1)^n r_2(n)q^n \tag{2.1.5}$$

where $r_2(n)$ counts the number of ways of writing $n=j^2+k^2$. Here we distinguish sign and permutation [so that, for example, $r_2(5)=8$ since $(\pm2)^2+(\pm1)^2=(\pm1)^2+(\pm2)^2$] and set $r_2(0):=1$. Now it is elementary that $r_2(2n)=r_2(n)$. (See Exercise 2.) It follows that

$$\theta_3^2(q)+\theta_4^2(q)=2\sum_{n=0}^{\infty} r_2(2n)q^{2n}=2\theta_3^2(q^2)\,. \tag{2.1.6}$$

Also, (2.1.4) and (2.1.6) allow us to solve for $\theta_3(q)\theta_4(q)$. We have

$$\begin{aligned}\theta_3(q)\theta_4(q)&=\tfrac12\,[\theta_3(q)+\theta_4(q)]^2-\tfrac12\,[\theta_3^2(q)+\theta_4^2(q)]\\ &=2\theta_3^2(q^4)-\theta_3^2(q^2)=\theta_4^2(q^2)\,.\end{aligned}$$

Thus

$$\frac{\theta_3^2(q)+\theta_4^2(q)}{2}=\theta_3^2(q^2) \tag{2.1.7i}$$

$$\sqrt{\theta_3^2(q)\theta_4^2(q)}=\theta_4^2(q^2) \tag{2.1.7ii}$$

which bears an obvious resemblance to the AGM. Similarly,

$$\begin{aligned}\theta_3^2(q)-\theta_3^2(q^2)&=\sum_{n=0}^{\infty} r_2(n)q^n-\sum_{n=0}^{\infty} r_2(2n)q^{2n}\\ &=\sum_{n=0}^{\infty} r_2(2n+1)q^{2n+1}\,.\end{aligned}$$

This last term may be rewritten as

$$\sum_{n=0}^{\infty} r_2(2n+1)q^{2n+1}=\sum_{\substack{k,m=-\infty\\ k+m \text{ odd}}}^{\infty} q^{m^2+k^2}$$

which, on setting $k=i-j$ and $m=i+j+1$, gives

$$\sum_{i,j=-\infty}^{\infty}(q^2)^{(i+1/2)^2+(j+1/2)^2}=\theta_2^2(q^2)\,.$$

Hence

$$\theta_3^2(q^2)+\theta_2^2(q^2)=\theta_3^2(q)\,. \tag{2.1.8}$$

This combines with (2.1.7i) to produce

$$\theta_3^2(q^2)-\theta_2^2(q^2)=\theta_4^2(q) \tag{2.1.9}$$

and these last two and (2.1.7ii) yield Jacobi's identity

$$\theta_3^4(q)=\theta_4^4(q)+\theta_2^4(q)\,. \tag{2.1.10}$$

Now set $k:=k(q):=\theta_2^2(q)/\theta_3^2(q)$. Then (2.1.10) shows that $k'=\theta_4^2(q)/\theta_3^2(q)$. If we return to (2.1.7) and set $a_n:=\theta_3^2(q^{2^n})$ and $b_n:=\theta_4^2(q^{2^n})$ we observe that a_n and b_n satisfy the AGM iteration. Moreover, since $\theta_3(0)=1$, the limit is 1. Thus

$$M(\theta_3^2(q),\theta_4^2(q))=1\,. \tag{2.1.11}$$

We recast these last observations in:

Theorem 2.1

Let $0<k<1$ be given. The AGM satisfies

$$M(1,k')=\theta_3^{-2}(q) \qquad \text{for} \qquad k'=\theta_4^2(q)/\theta_3^2(q) \tag{2.1.12}$$

where q is the unique solution in $(0,1)$ to $k=\theta_2^2(q)/\theta_3^2(q)$. In particular,

$$K(k)=\frac{\pi}{2}\,\theta_3^2(q)\,. \tag{2.1.13}$$

Proof. This follows from the previous discussion and Theorem 1.1. The uniqueness of q will be obvious from the results of Section 3.1, which will show that θ_4 decreases and θ_3 increases on $(0,1)$. □

The results of Theorem 2.1 remain true more generally in the complex plane. This is discussed in Exercise 4.

Comments and Exercises

The solution of the AGM in theta function terms can be found in Gauss

[1866]. The systematic investigation of theta functions in the context of elliptic function theory originates in Jacobi's masterpiece *Fundamenta Nova Theoriae* [1829].

While we have given a number-theoretically motivated development, it is possible to give a very elegant formal verification. (See Exercise 1.) This technique, used frequently by Liouville, is discussed in detail in Bell [27].

1. a) Let $f: \mathbb{Z}\times\mathbb{Z}\to\mathbb{R}$. Establish the formal identity

$$\sum_{m,n=-\infty}^{\infty} f(m,n)=\sum_{l,k=-\infty}^{\infty} f(l+k,l-k)+\sum_{l,k=-\infty}^{\infty} f(l+k,l-k-1) \tag{2.1.14}$$

valid whenever both terms on the right-hand side converge.

b) Apply (2.1.14) to $q^{m^2+n^2}$, $(-1)^{m+n}q^{m^2+n^2}$, and $(-1)^m q^{m^2+n^2}$ to derive (2.1.8), (2.1.9), and (2.1.7*ii*) respectively.

c) Hence rederive (2.1.7) and (2.1.10).

2. Prove that $r_2(n)=r_2(2n)$. *Hint*: $2a^2+2b^2=(a+b)^2+(a-b)^2$.

3. a) Show that the downward transformation [Theorem 1.2(b)] sends $k(q)$ to $\lambda(q):=k(q^2)$. Precisely,

$$\frac{1-k'}{1+k'}=\frac{\theta_3^2(q)-\theta_4^2(q)}{\theta_3^2(q)+\theta_4^2(q)}=\frac{\theta_2^2(q^2)}{\theta_3^2(q^2)}=\lambda\,. \tag{2.1.15}$$

b) Show that the corresponding transformation for K [Theorem 1.2(*b*)] is

$$\theta_3^2(q^2)=\left[\frac{1+\theta_4^2(q)/\theta_3^2(q)}{2}\right]\theta_3^2(q)\,. \tag{2.1.16}$$

4. Show that (2.1.12) is valid for complex q with $|q|<1$. Precisely,

$$M\left(1,\frac{\theta_4^2(q)}{\theta_3^2(q)}\right)=\theta_3^{-2}(q)$$

for such q. [That $\theta_3(q)$ does not vanish will be apparent from Section 3.1.]

2.2 *POISSON SUMMATION*

A most analytically accessible route to the behaviour of the AGM lies in the *Poisson summation formula*, which we now describe. We then give some examples of its use before returning in the next section to its relationship with the AGM. The formula we need is:

Theorem 2.2

Let f be a nonnegative function, increasing on $(-\infty,0]$ and decreasing on $[0,\infty)$. Assume that $\int_{-\infty}^{\infty} f(x)\,dx$ exists as an improper Riemann integral. Then, for each x in $\mathbb{R}$,

$$\sum_{n=-\infty}^{\infty}\frac{f(n+x+)+f(n+x-)}{2}=\sum_{k=-\infty}^{\infty} e^{2\pi ikx}\int_{-\infty}^{\infty} f(t)\,e^{-2\pi ikt}\,dt \tag{2.2.1}$$

each series being absolutely convergent.

Proof. A complete proof may be found in Apostol [74, pp. 332–333]. In essence one considers the function $F(x):=\sum_{n=-\infty}^{\infty} f(n+x)$, which under the given hypotheses is of bounded variation on compact intervals, and which is, by construction, periodic. The left-hand side of (2.2.1) is merely the average $[F(x+)+F(x-)]/2$, while the right-hand side is obtained by computing the Fourier coefficients for F and regrouping. □

EXAMPLE 2.1. We apply the formula to f given by

$$f(x):=\begin{cases} e^{-yx} & x\geq 0\,,\\ 0 & x<0\,,\end{cases}\qquad y>0\,.$$

The right-hand side becomes

$$\sum_{k=-\infty}^{\infty}\frac{e^{2\pi ikx}}{y+2\pi ik}=\frac{1}{y}+2\sum_{k=1}^{\infty}\frac{y\cos(2\pi kx)+(2\pi k)\sin(2\pi kx)}{y^2+(2\pi k)^2}$$

and the left-hand side becomes

$$\sum_{n>-x} e^{-y(n+x)}+\begin{cases}\frac{1}{2} & x\in\mathbb{Z}\\ 0 & \text{otherwise}\end{cases}.$$

If $x:=0$, we derive

$$\frac{1}{2}+\frac{1}{e^y-1}=\frac{1}{y}+2y\sum_{k=1}^{\infty}\frac{1}{y^2+(2\pi k)^2}$$

which yields

$$\pi\coth(\pi x)=\frac{1}{x}+2x\sum_{n=1}^{\infty}\frac{1}{x^2+n^2} \tag{2.2.2}$$

on replacing y by $2\pi x$.

If $x:=\frac{1}{2}$, we derive

$$\pi\,\mathrm{cosech}\,(\pi x)=\frac{1}{x}+2x\sum_{n=1}^{\infty}\frac{(-1)^n}{x^2+n^2}\,. \tag{2.2.3}$$

By elementary analyticity considerations, (2.2.2) and (2.2.3) remain valid in the complex plane and produce the classical formulae for cot, cosec, and so on. (See Exercise 1.)

EXAMPLE 2.2. This time apply the formula with

$$f(x) := e^{-sx^2\pi} \qquad s > 0 .$$

Then (2.2.1) becomes

$$\sum_{n=-\infty}^{\infty} e^{-s(n+x)^2\pi} = \sum_{k=-\infty}^{\infty} e^{2\pi ikx} \int_{-\infty}^{\infty} e^{-st^2\pi - 2\pi kit}\, dt .$$

Now the integral on the right is

$$2\int_0^{\infty} e^{-s\pi t^2} \cos(2\pi kt)\, dt = \frac{2}{\sqrt{s\pi}} F\left(\sqrt{\frac{\pi}{s}}\, k\right)$$

where

$$F(y) := \int_0^{\infty} e^{-x^2} \cos(2xy)\, dx = \frac{\sqrt{\pi}}{2} e^{-y^2} . \tag{2.2.4}$$

(See Exercise 2.) Thus we deduce

$$\sum_{n=-\infty}^{\infty} e^{-s(n+x)^2\pi} = s^{-1/2} \sum_{k=-\infty}^{\infty} e^{2\pi ikx} e^{-\pi k^2/s} . \tag{2.2.5}$$

Again, analyticity considerations show that (2.2.5) holds for $\operatorname{re}(s) > 0$. This is a general form of the *theta transformation formula*. For future reference we make the notational agreement that $\theta_i(s) := \theta_i(e^{-\pi s})$ and observe that for $x := 0$, (2.2.5) can be written as

$$\sqrt{s}\theta_3(s) = \theta_3(s^{-1}) . \tag{2.2.6}$$

Note that for large s the sum $\sqrt{s}\theta_3(s)$ converges much more rapidly than $\theta_3(s^{-1})$. For example, if $s := 100$, $\theta_3(0.01)$ and $10 + 20e^{-100\pi}$ coincide through more than 500 digits.

Comments and Exercises

The result of (2.2.1) was known to Poisson by 1827. With $x := 0$ he had obtained the formula in 1823. Equation (2.2.5) was first obtained by Jacobi using elliptic function theory in 1828.

1. Establish the formulae

a) $$\frac{\pi}{\sin(\pi z)} = \frac{1}{z} + \sum_{n=1}^{\infty} \frac{(-1)^n 2z}{z^2 - n^2}$$

b) $$\frac{\pi}{\cos(\pi z)} = \sum_{n=0}^{\infty} \frac{(-1)^{n+1}(2n+1)}{z^2 - (n+\frac{1}{2})^2}$$

c) $$\pi \cot(\pi z) = \frac{1}{z} + \sum_{n=1}^{\infty} \frac{2z}{z^2 - n^2}$$

d) $$\sin(\pi z) = \pi z \prod_{n=1}^{\infty} \left(1 - \frac{z^2}{n^2}\right).$$

2. Establish (2.2.4) by showing that

$$\dot{F}(y) + 2yF(y) = 0$$

and using $F(0) = \sqrt{\pi}/2$. (See Exercise 3 of Section 1.6.)

3. Let $I(s, y) := \int_{-\infty}^{\infty} e^{-s\pi t^2 - 2\pi yt}\, dt$. Evaluate $I(s, y)$ for real s, y by completing the square. By analytic continuation $I(s, ik) = s^{-1/2} e^{-\pi k^2/s}$.

4. Recall that the *Laplace transform* is defined by

$$F(y) := \int_0^{\infty} e^{-yt} f(t)\, dt .$$

Provided that $f(t) = O(e^{bt})$ as $t \to \infty$, F will be analytic for $\operatorname{re}(y) > b$. Show that the Laplace transform of (2.2.5) with $x := 0$ produces (2.2.2). This entails evaluating integrals of the form

$$F(a, b) := \int_0^{\infty} e^{-[a^2 t + b^2/t]}\, t^{-1/2}\, dt .$$

This is a special case of a Bessel function transform which can be evaluated explicitly as $F(a, b) = (\sqrt{\pi}/a)\, e^{-2ba}$ by substituting $s^2 := t$ and $v := b/s - as$. (Various extensions and related matters are discussed in Bellman [61].) In principle, therefore, one can derive (2.2.5) as an inverse Laplace transform of the derivative of the product form of sin given in Exercise 1d).

5. Let f be nonnegative, continuous, decreasing, and Riemann integrable on $[0, \infty)$. Let

$$g(y) := \sqrt{\frac{2}{\pi}} \int_0^{\infty} f(x) \cos(xy)\, dx .$$

Show that

$$\sqrt{\alpha}\left[\frac{1}{2}f(0)+\sum_{m=1}^{\infty}f(m\alpha)\right]=\sqrt{\beta}\left[\frac{1}{2}g(0)+\sum_{n=1}^{\infty}g(n\beta)\right]$$

whenever $\alpha, \beta > 0$ satisfy $\alpha\beta = 2\pi$. Deduce that

$$\sqrt{\alpha}\left[\frac{1}{2}+\sum_{m=1}^{\infty}e^{-\alpha^2m^2/2}\right]=\sqrt{\beta}\left[\frac{1}{2}+\sum_{n=1}^{\infty}e^{-\beta^2n^2/2}\right].$$

(Exercises 2 and 5 follow Apostol [74].)

2.3 *POISSON SUMMATION AND THE AGM*

We commence by specializing (2.2.5). Setting $x := 0$ produces

(2.3.1) $$\sqrt{s}\,\theta_3(e^{-s\pi})=\theta_3(e^{-\pi/s})$$

while $x := \frac{1}{2}$ gives

(2.3.2) $$\sqrt{s}\,\theta_2(e^{-s\pi})=\theta_4(e^{-\pi/s})$$

and dually on setting $s = s^{-1}$,

(2.3.3) $$\sqrt{s}\,\theta_4(e^{-s\pi})=\theta_2(e^{-\pi/s})$$

where $\operatorname{re}(s) > 0$. On dividing (2.3.2) by (2.3.1) we have

(2.3.4) $$k(e^{-\pi s})=k'(e^{-\pi/s})\,.$$

From Theorem 2.1 we see that

$$M(1,k)=\theta_3^{-2}(e^{-\pi/s})\qquad q:=e^{-\pi s}\,.$$

Thus

(2.3.5) $$\pi\,\frac{M(1,k')}{M(1,k)}=\pi\,\frac{\theta_3^2(e^{-\pi/s})}{\theta_3^2(e^{-\pi s})}=\pi s=-\log q$$

on using Theorem 2.1 and (2.3.1) again. This produces the following fundamental theorem.

Theorem 2.3

For all k in $(0, 1)$,

(*a*) $$\pi\,\frac{M(1,k')}{M(1,k)}=-\log q\qquad k=\frac{\theta_2^2(q)}{\theta_3^2(q)}\qquad k'=\frac{\theta_4^2(q)}{\theta_3^2(q)}$$

and so

(*b*) $$\pi\,\frac{K'(k)}{K(k)}=-\log q\,.$$

Proof. We have established (*a*) and (*b*) follows from our identification of $M(1, k')$ and $\pi/(2K(k))$. This second equation is often written as $q = e^{-\pi K'/K}$ and q is called the *nome* associated with k. In principle it solves the inversion problem for q in terms of k. □

We know that $k = \theta_2^2(q)/\theta_3^2(q) = 4\sqrt{q} + O(q)$ as q tends to zero from above. Theorem 2.3(*a*) and this information show that since $M(1, k')$ tends to 1 as k tends to zero,

(2.3.6) $$\lim_{k\to0^+}\left[\frac{\pi}{2M(1,k)}-\log\left(\frac{4}{k}\right)\right]=0$$

which reproduces the asymptotic of Exercise 4 of Section 1.3. As we shall see (Exercise 1), we can derive the exact asymptotic (1.3.10) from these considerations.

Now consider the AGM iteration commencing with $a_0 := 1$ and $b_0 := k'$. Then as we saw in Section 1, $b_n/a_n = k'(q^{2^n})$ and $c_n/a_n = k(q^{2^n})$. Hence

(2.3.7) $$\lim_{n\to\infty}2^{-n}\log\left(\frac{4a_n}{c_n}\right)=\frac{\pi}{2}\,\frac{M(1,k')}{M(1,k)}\,.$$

In Exercise 2 one establishes that the differential identity

(2.3.8) $$2^{-n}b_n^{-2}d\log\left(\frac{a_n}{c_n}\right)=b_0^{-2}d\log\left(\frac{a_0}{c_0}\right)$$

holds. It follows from (2.3.5) and (2.3.7) that

$$\pi_n := 2^{1-n}\,\frac{d}{ds}\log\left(\frac{a_n}{c_n}\right)\to\pi$$

and from (2.3.8),

$$\pi_n=\frac{b_n^2\pi_0}{b_0^2}\qquad\text{while}\qquad \pi_0=-\frac{2}{k}\,\frac{dk}{ds}\,.$$

Since b_n tends to $M(1, k')$, we have established that

$$\frac{dk}{ds} = -\frac{\pi}{2}\frac{kk'^2}{M(1,k')^2} = -\frac{2}{\pi}kk'^2K^2 \tag{2.3.9}$$

and since $s = -\pi^{-1}\log q$,

$$\frac{dk}{dq} = \frac{1}{2q}\frac{kk'^2}{M(1,k')^2} = \frac{2kk'^2K^2}{q\pi^2}. \tag{2.3.10}$$

Rewriting k, k', and K in (2.3.9) in theta terms produces

$$\frac{\dot\theta_3}{\theta_3} - \frac{\dot\theta_2}{\theta_2} = \frac{\pi}{4}\theta_4^4. \qquad \text{(w.r.t.}s\text{)*} \tag{2.3.11}$$

Differentiation of (2.3.1) and (2.3.3) yields

$$s^2\dot\theta_3(s) + \frac{s}{2}\theta_3(s) = -s^{-1/2}\dot\theta_3(s^{-1}) \qquad \text{(w.r.t.}s\text{)} \tag{2.3.12}$$

$$s^2\dot\theta_4(s) + \frac{s}{2}\theta_4(s) = -s^{-1/2}\dot\theta_2(s^{-1}). \qquad \text{(w.r.t.}s\text{)} \tag{2.3.13}$$

On using (2.3.1) and (2.3.2) again we deduce that

$$s\frac{\dot\theta_3}{\theta_3}(s) + s^{-1}\frac{\dot\theta_3}{\theta_3}(s^{-1}) = -\frac{1}{2} = s\frac{\dot\theta_4}{\theta_4}(s) + s^{-1}\frac{\dot\theta_2}{\theta_2}(s^{-1}). \tag{2.3.14}$$

Now, since $s^2\theta_4^4(s) = \theta_2^4(s^{-1})$, this shows that

$$\frac{\dot\theta_4}{\theta_4} - \frac{\dot\theta_3}{\theta_3} = \frac{\pi}{4}\theta_2^4 \qquad \text{(w.r.t.}s\text{)} \tag{2.3.15}$$

is equivalent to (2.3.11). Finally, adding (2.3.11) and (2.3.15) gives

$$\frac{\dot\theta_4}{\theta_4} - \frac{\dot\theta_2}{\theta_2} = \frac{\pi}{4}\theta_3^4 \qquad \text{(w.r.t.}s\text{)} \tag{2.3.16}$$

on using (2.1.10).

We can now also express E in terms of theta functions. We have from (1.3.13),

$$E - K = kk'^2\frac{dK}{dk} - k^2K = -\frac{\pi}{K}\left[\frac{1}{2K}\frac{dK}{ds} + \frac{k^2K^2}{\pi}\right]$$

because of (2.3.9). Hence

*Differentiation with respect to s.

$$E - K = -\frac{\pi}{K}\left[\frac{\dot\theta_3}{\theta_3} + \frac{\pi}{4}\theta_2^4\right] \qquad \text{(w.r.t.}s\text{)}$$

and

$$E = K - \frac{\pi}{K}\frac{\dot\theta_4}{\theta_4}. \qquad \text{(w.r.t.}s\text{)} \tag{2.3.17}$$

Similarly

$$E' - K' = \frac{\pi}{2K} + \frac{\pi K'}{K^2}\frac{\dot\theta_2}{\theta_2} \qquad \text{(w.r.t.}s\text{)}$$

and

$$E' = \frac{\pi}{2K} + \frac{\pi K'}{K^2}\frac{\dot\theta_4}{\theta_4}. \qquad \text{(w.r.t.}s\text{)} \tag{2.3.18}$$

Comments and Exercises

1. a) Observe that $k = 4\sqrt{q}f(q)$ with f analytic for $|q| < 1$ and $f(0) = 1$. Standard real reversion arguments show that for $0 < k < 1$,

$$\sqrt{q} = \frac{k}{4}g(k^2)$$

where g is (real) analytic with $g(0) = 1$. Show that

$$K'(k) = \frac{2}{\pi}K(k)\left[\log\left(\frac{4}{k}\right) + h(k)\right] \tag{2.3.19}$$

where $h(0) = 0$ and h is analytic.

b) Observe that the right-hand side of (1.3.10) and K' both solve (1.3.8). Moreover, both can be expressed in the form of the right-hand side of (2.3.19). Deduce that (1.3.10) holds.

2. a) Show that $2^{-n}b_n^{-2}\boldsymbol{d}\log(a_n/c_n)$ is independent of n.

b) From a) deduce that $2^{-n}c_n^{-2}\boldsymbol{d}\log(b_n/a_n)$ is independent of n.

c) Use a) and b) to show that $2^{-n}a_n^{-2}\boldsymbol{d}\log(b_n/c_n)$ is independent of n.

d) Show that all three coincide with $b_0^{-2}\boldsymbol{d}\log(a_0/c_0)$. This again is due to Gauss.

3. a) Establish (2.3.18) by using (2.3.16).

b) Observe that (2.3.18) and (2.3.17) immediately give another proof of Legendre's relation.

4. a) Show that $\theta_2(e^{-\pi}) = \theta_4(e^{-\pi})$.

b) Show that $4\pi = (\Sigma_{n=-\infty}^{\infty} e^{-n^2\pi})/(\Sigma_{n=-\infty}^{\infty} n^2 e^{-n^2\pi})$.
c) Let $r_k(n)$ give the number of distinct representations of n as a sum of k squares. Show that

$$4\pi = \left(\sum_{n=0}^{\infty} kr_k(n)\, e^{-n\pi}\right)\bigg/\left(\sum_{n=0}^{\infty} nr_k(n)\, e^{-n\pi}\right).$$

Hint: Take the kth power of (2.3.1) and differentiate.

All of results in this section can be derived without Poisson summation as the following exercises show.

5. Derive (2.3.7) by combining Exercise 1e) of Section 1.4 and Exercise 4b) of Section 1.3. This can also be found in Gauss [1866], but not apparently in later nineteenth-century authors. (See Borwein and Borwein [84*a*] and King [24].)
6. Use $k \sim 4\sqrt{q}$ to rederive Theorem 2.3 from Theorem 1.1.
7. Observe that Theorem 2.3(*a*) and Theorem 2.1 show (2.3.1) and (2.3.4). Hence deduce (2.3.2) and (2.3.3). Thus we have established the θ transformation formulae [(2.3.1) to (2.3.3)] directly from the AGM.
8. Suppose that in (2.3.7) the 4 is omitted. Show that the convergence, which was quadratic, is now linear. Of course the limit is unchanged.

2.4 THE DERIVED ITERATION AND SOME CONVERGENCE RESULTS

It is generally the case with AGM related approximations that it is relatively easy to establish the convergence rate and much harder to determine to what the given iteration converges. We now consider various preparatory convergence results. In the next section these will be used to produce two surprising algorithms for π.

Motivated by the fact that $\sqrt{2}K(1/\sqrt{2})\dot{K}(1/\sqrt{2}) = \pi$ (Exercise 2 of Section 1.6), we commence by computing $\dot{K}$. If we consider the AGM sequence with $a_0 := 1$ and $b_0 := k$, it is apparent that a_n and b_n viewed as functions of k converge uniformly and analytically to $M(1, k)$. It follows that the derived iterations $\dot{a}_n$ and $\dot{b}_n$ converge to $\dot{M}(1, k)$. Since $M(1, k) = \pi/2K'(k)$, we see that

$$\dot{M}(1, k) = \frac{\pi}{2}\frac{k}{k'}\frac{\dot{K}(k')}{K^2(k')} \tag{2.4.1}$$

on noting that $(dK'/dk)(k) = -(k/k')(dK/dk)(k')$. Equivalently,

$$\dot{K}(k') = \frac{\pi}{2}\frac{k'}{k}\frac{\dot{M}(1, k)}{M^2(1, k)}\,. \tag{2.4.2}$$

Now the derived iteration is

$$\dot{a}_{n+1} = \frac{\dot{a}_n + \dot{b}_n}{2} \qquad \dot{b}_{n+1} = \frac{\dot{a}_n\sqrt{b_n/a_n} + \dot{b}_n\sqrt{a_n/b_n}}{2}\,. \tag{2.4.3}$$

Since b_n/a_n converges quadratically to 1, it is easy to show directly that $\dot{a}_n$ and $\dot{b}_n$ converge quadratically to $\dot{M}(1, k)$ for $0 < k < 1$. Moreover $\dot{b}_n$ decreases and $\dot{a}_n$ increases, at least eventually (Exercise 1). For our purposes we will generally consider the *Legendre forms* $x_n := a_n/b_n$ and $y_n := \dot{b}_n/\dot{a}_n$. Then

$$x_{n+1} = \frac{\sqrt{x_n} + 1/\sqrt{x_n}}{2} \qquad y_{n+1} = \frac{y_n\sqrt{x_n} + 1/\sqrt{x_n}}{y_n + 1} \tag{2.4.4}$$

where $x_0 := k^{-1}$, $y_1 := \sqrt{x_0}$, and y_0 is undefined. Moreover,

$$1 \le x_{n+1} \le y_{n+1} \le \sqrt{x_n} \le x_n\,. \tag{2.4.5}$$

(See Exercise 2.) We also have

$$x_{n+1} - 1 = \frac{(x_n - 1)^2}{2\sqrt{x_n}(1 + \sqrt{x_n})^2} \le \frac{1}{8}(x_n - 1)^2$$

and

$$y_{n+1} - 1 = \frac{(y_n - 1)(x_n - 1)}{(y_n + 1)(\sqrt{x_n} + 1)} + \frac{2(x_{n+1} - 1)}{y_n + 1}$$
$$\le \tfrac{1}{4}(y_n - 1)^2 + \tfrac{1}{8}(x_n - 1)^2 \le \tfrac{3}{8}(y_n - 1)^2$$

so that for $n \ge 1$

$$x_{n+1} - 1 \le \tfrac{1}{8}(x_n - 1)^2 \tag{2.4.6i}$$

$$y_{n+1} - 1 \le \tfrac{3}{8}(y_n - 1)^2\,. \tag{2.4.6ii}$$

This establishes the quadratic convergence of x_n and y_n to 1. From (2.4.1), (2.4.2), and the previous discussion it is now apparent that

$$\pi = 2\sqrt{2}\,\frac{M^3(1, 1/\sqrt{2})}{\dot{M}(1, 1/\sqrt{2})} \tag{2.4.7}$$

and since both M and $\dot{M}$ are quadratically computable, so is π. In the next section we turn this identity into an explicit algorithm.

Comments and Exercises

1. Show that $\dot{a}_n$ and $\dot{b}_n$ defined by (2.4.3) converge quadratically to $\dot{M}(1, k)$, by showing that $\dot{a}_n$ increases and $\dot{b}_n$ decreases. Then show $\dot{b}_n - \dot{a}_n \le (\sqrt{x_{n-1}} - 1)/2$. For this to hold for all n, assume $x_0 \le 3$.

2. Establish (2.4.4) and (2.4.5).

3. a) Use $x_n = \theta_3^2(q^{2^n})/\theta_4^2(q^{2^n})$ to show that $x_n \sim 1 + 8e^{-2^n\pi(K/K')(x_0^{-1})}$ as $n \to \infty$.
   b) Show that $c_n \le 4a_n e^{-2^{n-1}\pi(K/K')(x_0^{-1})} := \delta_n$, and that $c_n \sim \delta_n$ as $n \to \infty$.

4. Show that with $a_0 := 1$ and $b_0 := k$,

$$\dot{K}(k') = \frac{\pi}{2}\frac{k'}{k}\lim_{n\to\infty}\frac{\dot{a}_n}{b_n^2}.$$

Hence deduce that with x_n and y_n, as in (2.4.4),

$$\dot{K}(k') = \frac{\pi}{4}\frac{k'}{k^2}\prod_{n=1}^{\infty}\frac{1+y_n}{2x_n}.$$

In particular with $x_0 := \sqrt{2}$ and $y_1 := 2^{1/4}$,

$$\prod_{n=1}^{\infty}\frac{1+y_n}{2x_n} = \frac{4\Gamma^2(\frac{3}{4})}{\pi^{3/2}} = \frac{8\sqrt{\pi}}{\Gamma^2(\frac{1}{4})}.$$

5. Show that

$$M\left(1, \frac{1}{\sqrt{2}}\right) = \pi^{-1/2}\Gamma^2\left(\frac{3}{4}\right) \quad \text{and} \quad \dot{M}\left(1, \frac{1}{\sqrt{2}}\right) = 2\sqrt{2}\pi^{-5/2}\Gamma^6\left(\frac{3}{4}\right).$$

2.5 *TWO ALGORITHMS FOR* π

The systematic use of the derived AGM leads directly to quadratic algorithms for π.

Algorithm 2.1

Let $x_0 := \sqrt{2}$, $\pi_0 := 2 + \sqrt{2}$, and $y_1 := 2^{1/4}$. Define

(i) $x_{n+1} := \frac{1}{2}\left(\sqrt{x_n} + \frac{1}{\sqrt{x_n}}\right)$ $\quad n \ge 0$

(ii) $y_{n+1} := \dfrac{y_n\sqrt{x_n} + 1/\sqrt{x_n}}{y_n + 1}$ $\quad n \ge 1$

(iii) $\pi_n := \pi_{n-1}\dfrac{x_n + 1}{y_n + 1}$ $\quad n \ge 1$.

Then π_n decreases monotonically to π. Moreover, for $n \ge 0$,

(2.5.1) $$\tfrac{3}{2}(y_{n+1} - x_{n+1}) \le \pi_n - \pi \le \tfrac{7}{4}(y_{n+1} - x_{n+1})$$

(2.5.2) $$\pi_{n+1} - \pi \le \frac{1}{10}(\pi_n - \pi)^2$$

and, for $n \ge 2$,

(2.5.3) $$\pi_n - \pi < 10^{-2^{n+1}}.$$

Proof. We first establish the limit. This follows from (2.3.7) (see Exercise 1) or from (2.4.7) as we now indicate. Let $\pi_n := 2\sqrt{2}b_{n+1}^2 a_{n+1}/\dot{a}_{n+1}$ where $a_0 := 1$ and $b_0 := 1/\sqrt{2}$. Then by (2.4.7) of the previous section, $\pi_n \to \pi$. From (2.4.4) we have

$$\frac{\pi_n}{\pi_{n-1}} = \frac{(b_{n+1}/b_n)^2(a_{n+1}/a_n)}{\dot{a}_{n+1}/\dot{a}_n} = \frac{1 + x_n}{1 + y_n}.$$

Moreover, $\pi_0 = 2 + \sqrt{2}$ and the algorithm converges to π as claimed. Since $y_n \ge x_n \ge 1$, it is obvious that π_n decreases. Let us observe that

(2.5.4) $$y_{n+1} - x_{n+1} = \frac{(y_n - 1)(x_n - 1)}{2\sqrt{x_n}(1 + y_n)} \le \frac{1}{8}(y_n - x_n)^2$$

provided that

$$\frac{x_n - 1}{y_n - 1} < 2 - \sqrt{3}.$$

Next

(2.5.5) $$\pi_n - \pi_{n+1} = \frac{\pi_n(y_{n+1} - x_{n+1})}{y_{n+1} + 1}.$$

Hence

$$\frac{\pi_n}{y_{n+1} + 1}(y_{n+1} - x_{n+1}) = \pi_n - \pi_{n+1} \le \frac{\pi_n}{2}(y_{n+1} - x_{n+1})$$

and

$$\pi_n - \pi \le \frac{\pi_n}{2}\sum_{k=1}^{\infty}(y_{n+k} - x_{n+k}) \le \frac{\pi_n}{2}\,\frac{y_{n+1} - x_{n+1}}{1 - \frac{1}{8}(y_{n+1} - x_{n+1})}.$$

Here we have used (2.5.4) and a geometric estimate. From the above

$$\pi_n - \pi \geq \frac{\pi}{y_{n+1}+1}(y_{n+1} - x_{n+1}) .$$

Thus, for $n > 0$, upon checking the early cases,

$$\frac{3}{2}(y_{n+1} - x_{n+1}) \leq \pi_n - \pi \leq \frac{7}{4}(y_{n+1} - x_{n+1}) \tag{2.5.6}$$

and with (2.5.4),

$$\pi_{n+1} - \pi \leq \frac{7}{4}(y_{n+2} - x_{n+2}) \leq \frac{7}{32}(y_{n+1} - x_{n+1})^2 \leq \frac{1}{10}(\pi_n - \pi)^2 .$$

Finally (2.5.3) follows from (2.5.2). □

The first nine iterations give 1, 3, 8, 19, 41, 83, 170, 345 and 694 digits of π. The 24th will produce more than 45 million digits at the expense of only a few hundred arithmetic operations. A more exact asymptotic will be derived in Chapter 5. (See Exercise 5.) Note also that the number of leading zeros of y_{n+1} gives the number of digits of agreement between π_n and π to within 1.

The second algorithm, based on an identity of Gauss [1866], was discovered by Brent [76*a*] and Salamin [76] independently.

Algorithm 2.2

Let $a_0 := 1$ and $b_0 := 1/\sqrt{2}$. Define

$$\pi_n := \frac{2a_{n+1}^2}{1 - \Sigma_{k=0}^{n} 2^k c_k^2}$$

where $c_n := \sqrt{a_n^2 - b_n^2} = c_{n-1}^2/4a_n$ and a_n and b_n are computed by the AGM iteration. Then π_n increases monotonically to π and satisfies

$$\pi - \pi_n \leq \frac{\pi^2 2^{n+4} e^{-\pi 2^{n+1}}}{M^2(1, 1/\sqrt{2})} \tag{2.5.7}$$

and

$$\pi - \pi_{n+1} \leq \frac{2^{-(n+1)}}{\pi^2}(\pi - \pi_n)^2 \tag{2.5.8}$$

Proof. This algorithm is based on the use of the second integral E rather than $\dot{K}$. With $k := 1/\sqrt{2}$ Legendre's relation is $(2E - K)K = \pi/2$. Combine this with Algorithm 1.2 of Section 1.4 to derive

$$\pi = \frac{2M^2(1, 1/\sqrt{2})}{1 - \Sigma_{k=0}^{\infty} 2^k c_k^2} \tag{2.5.9}$$

which on truncation shows that π_n converges to π. We leave the convergence estimates as Exercises 3 and 4. □

The first eight iterations produce 0, 3, 8, 19, 41, 84, 171 and 344 digits, which agrees extraordinarily well with the asymptotic.

Both of these algorithms generalize in many ways. (See Chapter 5.) At the moment we only exhibit two additional identities.

If we use the differential equation for K equation (1.3.13), we may rewrite Legendre's identity as

$$\frac{\pi}{2} = kk'^2(\dot{K}K' - K\dot{K}') . \tag{2.5.10}$$

[See equation (1.6.2).] With (2.4.2) we now derive

$$\frac{2}{\pi} = k'k^2 \frac{K'(k)}{K(k)} \frac{\dot{M}(1, k')}{M^3(1, k')} + kk'^2 \frac{K'(k')}{K(k')} \frac{\dot{M}(1, k)}{M^3(1, k)} \tag{2.5.11}$$

and, as in Algorithm 2.1, we can produce

$$\pi = \frac{2}{(1 - k')\dfrac{K'(k)}{K(k)} \displaystyle\prod_{n=1}^{\infty} \left(\frac{1 + y_n}{1 + x_n}\right) + (1 - k)\dfrac{K(k)}{K'(k)} \displaystyle\prod_{n=1}^{\infty} \left(\frac{1 + y_n^*}{1 + x_n^*}\right)} . \tag{2.5.12}$$

Here $x_0 := k'^{-1}$, $x_0^* := k^{-1}$, $y_1 := \sqrt{x_0}$, $y_1^* := \sqrt{x_0^*}$, and the iterations are given by (2.4.4). When $k := 1/\sqrt{2}$, (2.5.12) reduces exactly to Algorithm 2.1. Also whenever $K'(k)/K(k) = \sqrt{r}$ for rational r (a *singular value* of k), we can in principle find k algebraically, as we will see in Chapter 4. We already know of four such values of k. (Exercise 7.)

In a similar fashion we may use Algorithm 1.2 to substitute for both E and E' in Legendre's relation. This as observed in Salamin [76] produces

$$\pi = \frac{2M(1, k)M(1, k')}{1 - \Sigma_{n=0}^{\infty} 2^{n-1}(c_n^2 + c_n^{*2})} . \tag{2.5.13}$$

Again, c_n and c_n^* are computed from complementary AGM iterations. When $k := 1/\sqrt{2}$, this identity reduces to (2.5.9).

From (2.5.2) and (2.5.8) we observe explicitly that the corresponding algorithms converge quadratically. We are primarily interested in the cumulative error given by (2.5.3) and (2.5.7). We will say, informally, that any such algorithm allows for *quadratic* or *fast computation*. In similar fashion, we talk about mth-order computation if the cumulative error (i.e., digits correct) is of order m^n after n steps.

Comments and Exercises

Algorithm 2.1 is derived in Borwein and Borwein [84*a*] by the method of Exercise 1.

1. a) Differentiate (2.3.7) and apply (2.3.8) to establish that with $a_0 := 1$ and $b_0 := k'$,

$$\pi = \frac{2}{kk'^2} \lim_{n\to\infty} \frac{(a_n^* a_n)^2}{\dot{a}_n^* a_n - \dot{a}_n a_n^*}.$$

Here a_n^* as usual denotes the AGM iteration commencing with $b_0 := k$, and all derivatives are with respect to k.

b) Let $k := k' := 1/\sqrt{2}$ and observe that the previous formula reduces to (2.4.7).

2. a) Fill in the details in (2.5.3) to (2.5.6).

b) Show that

$$\lim_{n\to\infty} \frac{\pi_n - \pi}{y_{n+1} - 1} = \frac{\pi}{2}.$$

Note that while Algorithm 2.1 relies on evaluating $\dot{K}$, Algorithm 2.2 in fact relies on evaluating $\dot{E}$. Indeed (1.3.12) and Algorithm 1.2(*b*) combine to show that

$$\dot{E}(k) = -\frac{1}{k}\left(\sum_{n=0}^{\infty} 2^{n-1} c_n^2\right) K(k).$$

3. a) Use (2.3.7) to show that $(c_n/4a_n)^{1/2^{n-1}}$ increases monotonically and quadratically to q. This gives a quadratic algorithm for e^{π} on using $a_0 := 1$ and $b_0 := 1/\sqrt{2}$.

b) Show explicitly that, with $a_0 := 1$ and $b_0 := k'$,

(2.5.14) $$e^{\pi K'(k)/K(k)} = \frac{16}{k^2} \prod_{n=0}^{\infty} \left(\frac{a_{n+1}}{a_n}\right)^{2^{1-n}}.$$

4. As in Algorithm 2.2, show that

$$(2^n - 2^{-1}) \frac{\pi_{n+1}^2 c_{n+1}^2}{a_{n+2}^2} \le \pi_{n+1} - \pi_n \le \frac{\pi^2 2^n c_{n+1}^2}{M^2(1, 1/\sqrt{2})}.$$

Then deduce that

$$\pi_{n+1}^2\left(\frac{2^n - 2^{-1}}{a_{n+2}^2}\right) c_{n+1}^2 \le \pi - \pi_n \le \frac{\pi^2}{M^2(1, 1/\sqrt{2})} 2^{n+1} c_{n+1}^2.$$

Now use Exercise 3a) to show (2.5.7) and (2.5.8).

5. As in Exercise 4), show that in Algorithm 2.1 $\pi_n - \pi$ is of order $2^n e^{-\pi 2^{n+1}}$. Convergence proofs of this type can be found in detail in Salamin [76] and Borwein and Borwein [84*a*] with discussion of the asymptotics.

6. Prove (2.5.12).

7. Recall from Section 1.6 (see also Chapter 4) that

i) $K'\left(\frac{1}{\sqrt{2}}\right) = \sqrt{1} K\left(\frac{1}{\sqrt{2}}\right)$

ii) $K'(\sqrt{2} - 1) = \sqrt{2} K(\sqrt{2} - 1)$

iii) $K'\left(\frac{\sqrt{3} - 1}{2\sqrt{2}}\right) = \sqrt{3} K\left(\frac{\sqrt{3} - 1}{2\sqrt{2}}\right)$

iv) $K'(3 - 2\sqrt{2}) = \sqrt{4} K(3 - 2\sqrt{2})$.

Observe that for these values of k and k' (2.5.12) reduces to an algebraic combination of two infinite products. Equally (2.5.13) simplifies.

8. Establish the general identity of Gauss, Brent, and Salamin given as (2.5.13).

9. Use the quartic transformation to produce a quartically convergent infinite product for π. (See Exercise 3e) of Section 1.4.)

10. Show that with x_n and y_n as in Algorithm 2.1,

$$(\sqrt{2} + 2) \prod_{n=1}^{\infty} x_n \left(\frac{1 + x_n}{1 + y_n}\right) = \Gamma^4\left(\frac{3}{4}\right)\sqrt{2}$$

and

$$(\sqrt{2} + 2)^3 \prod_{n=1}^{\infty} x_n^{-1} \left(\frac{1 + x_n}{1 + y_n}\right)^3 = \frac{\Gamma^4(\frac{1}{4})}{\sqrt{32}}.$$

11. There are actually eight natural products implicit in (2.4.7). One can select either b_n or a_n ($\dot{b}_n$ or $\dot{a}_n$) for each of the means. While Algorithm 2.1 is the cleanest of these, it is not the best approximation.

a) Show that there are four decreasing and four increasing products.

b) Show that the two best approximations are given by $2\sqrt{2} b_n^3/\dot{a}_n$ and $2\sqrt{2} a_n^3/\dot{b}_n$.

c) Show that with x_n and y_n as in Algorithm 2.1,

$$2^{7/4}\prod_{m=1}^{n}\sqrt{x_m}\,\frac{2x_m}{1+y_m}\geq\pi\geq 2^{1/4}(\sqrt{2}+1)\prod_{m=1}^{n}\sqrt{x_m}\,\frac{y_m+y_mx_m}{1+y_mx_m}$$

with both products converging monotonically to π.

d) Similarly, produce a decreasing analogue to Algorithm 2.2.

12. The identity (2.5.14) can be found in Gauss [1866]. Show similarly the following identity due to Jacobi. (See King [24].)

$$\pi\,\frac{K'(k)}{K(k)}=\log\left(\frac{16k'}{k^2}\right)+3\sum_{n=1}^{\infty}2^{-n}\log\left(\frac{a_n}{b_n}\right)\qquad a_0:=1\quad b_0:=k'\,.$$

(2.5.15)

2.6 GENERAL THETA FUNCTIONS

Theta functions are more properly considered as a function of two variables—a parameter q and an analytic variable z. So far we have considered only special theta functions ($z=0$). In this section we sketch some relevant parts of the general theory. We write

(2.6.1)
$$\begin{aligned}
\theta_1(z,q)&:=\theta_1(z,t):=2q^{1/4}\sin z-2q^{9/4}\sin 3z\\
&\qquad+2q^{25/4}\sin 5z-\cdots\\
\theta_2(z,q)&:=\theta_2(z,t):=2q^{1/4}\cos z+2q^{9/4}\cos 3z\\
&\qquad+2q^{25/4}\cos 5z+\cdots\\
\theta_3(z,q)&:=\theta_3(z,t):=1+2q\cos 2z+2q^4\cos 4z\\
&\qquad+2q^9\cos 6z+\cdots\\
\theta_4(z,q)&:=\theta_4(z,t):=1-2q\cos 2z+2q^4\cos 4z\\
&\qquad-2q^9\cos 6z+\cdots
\end{aligned}$$

where $q=e^{\pi it}$ and $\mathrm{im}(t)>0$.

When $z=0$, then $\theta_1(0,q)=0$ and $\theta_j(0,q)=\theta_j(q)$ for $j=2,3,4$. When the precise value of q is unimportant, one writes $\theta_j(q)=\theta_j$ and $\theta_j(z,q)=\theta_j(z)$. When j is unimportant, one writes $\theta(z)$. It is straightforward to establish the following functional identities (Exercise 1):

(2.6.2)
$$\begin{aligned}
\theta_1(z)&=-\theta_2\left(z+\frac{\pi}{2}\right)=-iM\theta_3\left(z+\frac{\pi}{2}+\frac{\pi t}{2}\right)=-iM\theta_4\left(z+\frac{\pi t}{2}\right)\\
\theta_2(z)&=M\theta_3\left(z+\frac{\pi t}{2}\right)=M\theta_4\left(z+\frac{\pi}{2}+\frac{\pi t}{2}\right)=\theta_1\left(z+\frac{\pi}{2}\right)\\
\theta_3(z)&=\theta_4\left(z+\frac{\pi}{2}\right)=M\theta_1\left(z+\frac{\pi}{2}+\frac{\pi t}{2}\right)=M\theta_2\left(z+\frac{\pi t}{2}\right)\\
\theta_4(z)&=-iM\theta_1\left(z+\frac{\pi t}{2}\right)=iM\theta_2\left(z+\frac{\pi}{2}+\frac{\pi t}{2}\right)=\theta_3\left(z+\frac{\pi}{2}\right)
\end{aligned}$$

where the multiplier M is given by

(2.6.3)
$$M:=q^{1/4}e^{iz}\,.$$

From (2.6.2) or directly one has

(2.6.4)
$$\begin{aligned}
\theta_1(z)&=-\theta_1(z+\pi) &\quad \theta_1(z)&=-qe^{2iz}\theta_1(z+\pi t)\\
\theta_2(z)&=-\theta_2(z+\pi) & \theta_2(z)&=qe^{2iz}\theta_2(z+\pi t)\\
\theta_3(z)&=\theta_3(z+\pi) & \theta_3(z)&=qe^{2iz}\theta_3(z+\pi t)\\
\theta_4(z)&=\theta_4(z+\pi) & \theta_4(z)&=-qe^{2iz}\theta_4(z+\pi t)\,.
\end{aligned}$$

These identities show us that any theta function is entirely determined by its values on any fundamental parallelogram

$$P(z_0):=\{z\,|\,z=z_0+r_1\pi+r_2\pi t,\ 0\leq r_1,r_2\leq 1\}\,.$$

We assume as we may that the given function has no zeros on the boundary of $P(z_0)$. It is obvious that $z=0$ is a zero of $\theta_1(z)$ so that $\pi/2$, $\pi/2+\pi t/2$, and $\pi t/2$ are zeros of $\theta_2(z)$, $\theta_3(z)$ and $\theta_4(z)$, respectively. Moreover, (2.6.4) shows that $z_0+m\pi+n\pi t$ (m,n integral) is a zero of a theta function whenever z_0 is. We now show that each theta function has exactly one zero in each fundamental parallelogram. Thus we will have specified all the zeros above.

Consider the integral

$$N=\frac{1}{2\pi i}\int_{P(z_0)}\frac{\dot\theta(z)}{\theta(z)}\,dz$$

which gives the number of zeros of θ inside $P(z_0)$. Explicitly,

$$2\pi iN = \int_{z_0}^{z_0+\pi}\left[\frac{\dot\theta(z)}{\theta(z)} - \frac{\dot\theta(z+\pi t)}{\theta(z+\pi t)}\right]dz$$

$$- \int_{z_0}^{z_0+\pi t}\left[\frac{\dot\theta(z)}{\theta(z)} - \frac{\dot\theta(z+\pi)}{\theta(z+\pi)}\right]dz\,.$$

Now logarithmic differentiation of (2.6.4) shows that

(2.6.5) $$\frac{\dot\theta(z)}{\theta(z)} = \frac{\dot\theta(z+\pi)}{\theta(z+\pi)} = 2i + \frac{\dot\theta(z+\pi t)}{\theta(z+\pi t)}\,.$$

Thus $2\pi iN = 2\pi i$ and $N = 1$ as required.

The identities in (2.6.4) show that each θ_i/θ_j, $i \neq j$, is doubly periodic. In combination with our knowledge of the zeros of each θ_j we can painlessly apply Liouville's principle (bounded entire functions are constant) to establish many identities. We illustrate this with the following.

Proposition 2.1

(2.6.6) $$\theta_4^2(z)\theta_4^2 = \theta_3^2(z)\theta_3^2 - \theta_2^2(z)\theta_2^2\,.$$

Proof. Consider

$$f(z) := \frac{\theta_3^2(z)\theta_3^2 - \theta_2^2(z)\theta_2^2}{\theta_4^2(z)}\,.$$

By (2.6.4) $f(z)$ is doubly periodic with periods π and πt. Moreover $\theta_4^2(z)$ has a double zero at $\pi t/2$ in $P(0)$. Also (2.6.2) shows that $\theta_3^2(\pi t/2)\theta_3^2 = \theta_2^2(\pi t/2)\theta_2^2$. Thus f is elliptic with at most one simple pole in $P(0)$, and by Exercise 3a) of Section 1.7, f can have no poles. Hence f is constant, being bounded and analytic. Since $\theta_2(\pi/2) = 0$ and $\theta_3(\pi/2) = \theta_4$, $\theta_4(\pi/2) = \theta_3$, the constant must be θ_4^2 and (2.6.6) follows. □

Note that on letting $z = 0$ in (2.6.6), we recover (2.1.10): $\theta_3^4 = \theta_2^4 + \theta_4^4$.

It is a simple matter to recast Example 2.2 as the classical theta transformation formula.

Theorem 2.4

For z an arbitrary complex number and $\operatorname{im}(t) > 0$,

(2.6.7) $$\theta_3(z, t) = (-it)^{-1/2}\, e^{z^2/(\pi it)}\theta_3\left(\frac{z}{t}, -\frac{1}{t}\right).$$

Here one takes the principal square root. The proof is left as Exercise 3. It is equally simple to use the Jacobi triple-product of Chapter 3 to

produce product expressions for $\theta_j(z)$ (Exercise 4). Various other relationships are indicated in the exercises.

Comments and Exercises

There is a proliferation of notations for theta functions. We follow the most usual notations (used in Bellman [61]) and note that both Dickson [71, vol. 3, p. 93] and Whittaker and Watson [27] give tables of alternate notations. The abuse of functional notation, in particular the distinctions among θ_j, $\theta_j(q)$, $\theta_j(t)$, and $\theta_j(z)$, necessitates some caution. Both Bellman [61] and Whittaker and Watson [27] provide an accessible introduction to a considerable amount of material on theta functions.

1. Verify the identities of (2.6.2) and (2.6.4). Note that (2.6.2) shows that we can restrict attention to one theta function (say, θ_3) and lose no information.

2. Show using Liouville's principle that,

a) $\theta_2^2(z)\theta_4^2 = \theta_4^2(z)\theta_2^2 - \theta_1^2(z)\theta_3^2$

b) $\theta_3^2(z)\theta_4^2 = \theta_4^2(z)\theta_3^2 - \theta_1^2(z)\theta_2^2$

c) $\theta_3(z+w)\theta_3(z-w)\theta_3^2 = \theta_3^2(w)\theta_3^2(z) + \theta_1^2(w)\theta_1^2(z)$

d) $\theta_4(z+w)\theta_4(z-w)\theta_4^2 = \theta_4^2(w)\theta_4^2(z) - \theta_1^2(w)\theta_1^2(z)$

e) $\theta_1(z+w)\theta_4(z-w)\theta_2\theta_3 = \theta_1(z)\theta_4(z)\theta_2(w)\theta_3(w) + \theta_2(z)\theta_3(z)\theta_1(w)\theta_4(w)\,.$

Results of this kind are discussed in detail by Whittaker and Watson. Many are given in tabular form in Erdélyi et al. [53].

3. Establish Theorem 2.4.

4. Show that with $Q_0 := \prod_{n=1}^{\infty}(1-q^{2n})$,

i) $$\theta_3(z) = Q_0\prod_{n=1}^{\infty}(1+2q^{2n-1}\cos(2z)+q^{4n-2})$$

ii) $$\theta_1(z) = 2q^{1/4}Q_0\sin z\prod_{n=1}^{\infty}(1-2q^{2n}\cos(2z)+q^{4n})\,.$$

Establish similar identities for $\theta_2(z)$ and $\theta_4(z)$. Many variations are listed in Erdélyi et al. [53]. (This relies on Section 3.1.)

5. Use Exercise 4 to show that

i) $$\frac{\dot\theta_3(z)}{\theta_3(z)} = 4\sum_{n=1}^{\infty}\frac{(-1)^n q^n\sin(2nz)}{1-q^{2n}}$$

ii) $\log\left[\frac{\theta_3(z)}{\theta_3(0)}\right] = 4\sum_{n=1}^{\infty} \frac{(-1)^n q^n}{1-q^{2n}} \frac{\sin^2(nz)}{n}$

for $|\mathrm{im}(z)| < \frac{1}{2}\log|q|$.

6. One of the easy but important properties of theta functions is that they solve the one-dimensional heat or diffusion equation

$$\frac{\partial^2\theta(z,t)}{\partial z^2} = \frac{4i}{\pi}\frac{\partial\theta(z,t)}{\partial t}.$$

This provides a significant connection between the analytic properties of theta functions as functions of z and their number theoretic properties which revolve around the variable q. Various of these matters are pursued in Bellman [61] and Rademacher [73].

7. Bellman [61] gives an interesting functional equation approach to Theorem 2.4. Consider entire solutions f to

i) $f(z+\pi) = f(z)$
ii) $f(z+\pi t) = be^{-2iz}f(z)$

where b is an unspecified function of t independent of z. Suppose, temporarily, that f possesses an absolutely convergent Fourier expansion valid for all z:

$$f(z) := \sum_{n=-\infty}^{\infty} c_n e^{2niz}.$$

a) Show that $c_{n+1} = b^{-1}q^{2n}c_n$. Hence deduce that for $|q| = |e^{\pi it}| < 1$,

$$f(z) = c_0\left[1 + \sum_{n=-\infty}^{\infty} q^{n(n-1)}b^{-n}e^{2niz}\right]$$

is an analytic solution to i) and ii) and is unique up to choice of constant. When $q = b^{-1}$, we recover $\theta_3(z)$.

b) Show that any entire solution to i) and ii) has an absolutely convergent Fourier series. *Hint*: Use contour integration to show that for any integral k,

$$\left|\int_{-\pi/2}^{\pi/2} f(z)\, e^{-2inz}\, dz\right| \le e^{-2kn}\pi \max_{-\pi/2\le w\le\pi/2} |f(w-ik)|.$$

c) Use the uniqueness of solutions of i) and ii) to rederive Theorem 2.4. *Hint*: Show that both sides satisfy i) and ii). Then use Exercise 6 to normalize the equation.

There is also a considerable literature on multidimensional theta functions. (See Bellman [61].) Since they do not impinge on our main considerations, we say no more.

2.7 THE LANDEN TRANSFORMATION

We finish this chapter by deriving an expression for sn in terms of theta quotients and by relating this expression to the transformation of incomplete elliptic integrals. We begin with the classical Landen transformation in theta form.

Theorem 2.5

For all z and $\mathrm{im}(t) > 0$,

$$\text{(2.7.1)} \qquad \frac{\theta_3(z,t)\theta_4(z,t)}{\theta_4(2z,2t)} = \frac{\theta_3(0,t)\theta_4(0,t)}{\theta_4(0,2t)} = \frac{\theta_2(z,t)\theta_1(z,t)}{\theta_1(2z,2t)}.$$

Proof. As a function of z, $\theta_4(2z,2t)$ has zeros when $2z = \pi t + m\pi + 2n\pi t$ or when $z = m\pi/2 + (2n+1)\pi t/2$. This is exactly where $\theta_3(z,t)$ or $\theta_4(z,t)$ is zero. Again (2.6.4) shows that $f_t(z) := \theta_3(z,t)\theta_4(z,t)/\theta_4(2z,2t)$ is doubly periodic with periods π and πt. Thus Liouville's theorem shows that $f_t(z)$ is a constant with respect to z. The second equality follows on substituting $z + \pi t/2$ for z and using (2.6.2). □

To establish the existence and analyticity of sn in theta terms we begin with

$$\text{(2.7.2)} \qquad \frac{d}{dz}\frac{\theta_1(z)}{\theta_4(z)} = \theta_4^2\,\frac{\theta_2(z)\theta_3(z)}{\theta_4^2(z)}.$$

(See Exercise 1.) Now let $\rho := \theta_1(z)/\theta_4(z)$ and observe that

$$\text{(2.7.3)} \qquad \left(\frac{d\rho}{dz}\right)^2 = (\theta_2^2 - \rho^2\theta_3^2)(\theta_3^2 - \rho^2\theta_2^2).$$

(This relies on Exercises 2a) and 2b) of the previous section.) Then replacing z by $u\theta_3^{-2}$ and ρ by $y = \rho\theta_3/\theta_2$, we observe that, since $k^2 = \theta_2^4/\theta_3^4$,

$$\text{(2.7.4)} \qquad \left(\frac{dy}{du}\right)^2 = (1-y^2)(1-k^2y^2).$$

This is solved by

$$\text{(2.7.5)} \qquad \mathrm{sn}(u,k) := y = \frac{\theta_3}{\theta_2}\frac{\theta_1(u\theta_3^{-2})}{\theta_4(u\theta_3^{-2})}$$

or

$$\sqrt{k}\,\mathrm{sn}(u,k) = \frac{\theta_1(u\pi/2K)}{\theta_4(u\pi/2K)}$$

and then, in agreement with (1.7.1),

$$u = \int_0^{\mathrm{sn}(u,k)} \frac{dy}{\sqrt{(1-y^2)(1-k^2y^2)}}$$

which solves the inversion problem (at least for real k) for the given integral. We wish to have $\mathrm{cn}^2+\mathrm{sn}^2=1$ and $k^2\,\mathrm{sn}^2+\mathrm{dn}^2=1$, and it is appropriate to define

(2.7.6) $$\mathrm{cn}(u,k) := \frac{\theta_4}{\theta_2}\frac{\theta_2(u\theta_3^{-2})}{\theta_4(u\theta_3^{-2})} = \sqrt{\frac{k'}{k}}\,\frac{\theta_2}{\theta_4}\frac{(u\pi/2K)}{(u\pi/2K)}$$

(2.7.7) $$\mathrm{dn}(u,k) := \frac{\theta_4}{\theta_3}\frac{\theta_3(u\theta_3^{-2})}{\theta_4(u\theta_3^{-2})} = \sqrt{k'}\,\frac{\theta_3}{\theta_4}\frac{(u\pi/2K)}{(u\pi/2K)}\,.$$

(See Exercise 2.)

Finally we wish to recast Theorem 2.5 in elliptic function terms.

***Theorem 2.6* (*The Descending Landen Transform*)**

Let $0<\psi$ and $0<k<1$ be given. If

$$k_1 := \frac{1-k'}{1+k'}$$

and $0 \le \psi \le \psi_1$ is given by

$$\sin\psi_1 := \frac{(1+k')\sin\psi\cos\psi}{\sqrt{1-k^2\sin^2\psi}}$$

then

(2.7.8) $$(1+k')\int_0^{\psi}\frac{d\theta}{\sqrt{1-k^2\sin^2\theta}} = \int_0^{\psi_1}\frac{d\theta}{\sqrt{1-k_1^2\sin^2\theta}}$$

or

$$(1+k')F(\psi,k) = F(\psi_1,k_1)$$

where

$$F(\psi,k) := \int_0^{\psi}\frac{d\theta}{\sqrt{1-k^2\sin^2\theta}}$$

is the *incomplete elliptic integral* of the first kind.

Proof. From Theorem 2.5 we deduce

$$\frac{\theta_1(z,t)\theta_2(z,t)}{\theta_3(z,t)\theta_4(z,t)} = \frac{\theta_1(2z,2t)}{\theta_4(2z,2t)}\,.$$

In terms of sn, cn, and dn this becomes

$$\frac{k\,\mathrm{sn}(u,k)\,\mathrm{cn}(u,k)}{\mathrm{dn}(u,k)} = \sqrt{k_1}\,\mathrm{sn}(u_1,k_1)$$

where $u = z\theta_3^2(q)$ and $u_1 = 2z\theta_3^2(q^2)$ since $k_1 = \theta_2(q^2)/\theta_3(q^2)$.

Thus $k_1 = (1-k')/(1+k')$ and $u_1 = 2u\theta_3^2(q^2)/\theta_3^2(q) = (1+k')u$. Collecting information, we have

(2.7.9) $$u_1 = (1+k')u \qquad k_1 = \frac{1-k'}{1+k'} \qquad \mathrm{sn}(u_1,k_1) = (1+k')\frac{\mathrm{sn}\,\mathrm{cn}}{\mathrm{dn}}$$

since $kk_1^{-1/2} = 1+k'$. The change of variables $\sin\theta = \mathrm{sn}(u,k)$ and $\sin\theta_1 = \mathrm{sn}(u_1,k_1)$ now produces (2.7.8). □

Comments and Exercises

A profusion of information on the numerical use and derivation of various Landen transforms is given in King [24]. More bibliographic information is available in Watson [33] and in Whittaker and Watson [27].

1. Prove the differential equation (2.7.2) by showing that

$$\phi(z) := \frac{\dot\theta_1(z)\theta_4(z) - \dot\theta_4(z)\theta_1(z)}{\theta_2(z)\theta_3(z)}$$

is doubly periodic with periods π and $\pi t/2$ and that $\phi(z)$ has simple poles possibly only at $\pi/2$, $\pi/2+\pi t/2$, and translated points. Then show that $\phi(z+\pi t/2) = \phi(z)$, and hence relative to the periods π and $\pi t/2$, ϕ is doubly periodic with a single pole. Thus ϕ is constant.

2. a) Establish (2.7.5).

b) With cn and dn defined as in (2.7.6) and (2.7.7) show that $\mathrm{cn}^2+\mathrm{sn}^2=1$, $\mathrm{dn}^2+k^2\,sn^2=1$, and that $\mathrm{cn}(0)=\mathrm{dn}(0)=1$.

c) Show that $(d/du)\,\mathrm{sn}(u,k) = \mathrm{cn}(u,k)\,\mathrm{dn}(u,k)$.

d) Show that sn is strictly increasing on $(0,k)$ with $\mathrm{sn}(0,k)=0$ and $\mathrm{sn}(K,k)=1$. [You may find it convenient to use the product formulae for $\theta_1(z)$ and $\theta_4(z)$.]

e) Show that $\mathrm{dn}(K)=k'$.

f) Establish the double periodicity of $\mathrm{sn}(u,k)$, $\mathrm{cn}(u,k)$, and $\mathrm{dn}(u,k)$ with respect to u and verify the following table:

	Periods	Zeros	Poles	Residues
sn	$4K, 2iK'$	$2mK + 2niK'$	$2mK + (2n+1)iK'$	$(-1)^m/k$
cn	$4K, 2(K+iK')$	$(2m+1)K + 2niK'$	$2mK + (2n+1)iK'$	$(-1)^{m+1}i/k$
dn	$2K, 4iK'$	$(2m+1)K + (2n+1)iK'$	$2mK + (2n+1)iK'$	$(-1)^{n+1}i$

3. The ascending Landen transform is given by reversing the roles of k and k_1, ψ and ψ_1. Thus if

$$k_1 = \frac{2\sqrt{k}}{1+k}$$

and

$$\sin(2\psi_1 - \psi) = k \sin\psi \qquad \psi_1 \geq \psi$$

then

$$\frac{(1+k)}{2} F(\psi, k) = F(\psi_1, k_1)\,.$$

These transforms and their analogues for incomplete second and third integrals clearly lead to quadratic iterations which are studied in detail in King [24] without reference to theta functions. Note that if $\psi = \pi/2$, we recover the quadratic transformation for K.

a) Show that, in the notation of Theorem 2.6,

$$\cos\psi_1 = \frac{\cos^2\psi - k'\sin^2\psi}{\sqrt{1-k^2\sin^2\psi}}\,.$$

b) Hence show that

$$\sin(2\psi - \psi_1) = \frac{1-k'}{1+k'}\sin\psi_1 = k_1 \sin\psi_1\,.$$

c) Thus show that, if $k = 2\sqrt{k_1}/(1+k_1)$ and $\sin(2\psi - \psi_1) = k_1 \sin\psi_1$, then

$$F(\psi, k) = \frac{1+k_1}{2} F(\psi_1, k_1)\,.$$

Compare Exercise 5 of Section 1.4.

4. a) Show that if $u := 2Kx/\pi$, then

$$\mathrm{sn}(u,k) = 2q^{1/4}k^{-1/2}\sin(x)\prod_{n=1}^{\infty}\left[\frac{1-2q^{2n}\cos(2x)+q^{4n}}{1-2q^{2n-1}\cos(2x)+q^{4n-2}}\right].$$

b) Find similar expressions for cn and dn.

5. Combine Exercise 4a) and Theorem 2.6 to produce a quadratically converging approximation to $\mathrm{sn}(u, k)$ given one for $\sin x$.
6. Use (2.7.5) and Exercise 2 of Section 2.6 to show "the addition theorem"

$$\mathrm{sn}(u+v) = \frac{\mathrm{sn}(u)\,\mathrm{cn}(v)\,\mathrm{dn}(v) + \mathrm{sn}(v)\,\mathrm{cn}(u)\,\mathrm{dn}(u)}{1 - k^2\,\mathrm{sn}^2(u)\,\mathrm{sn}^2(v)}\,.$$

Obtain similar expressions for $\mathrm{cn}(u+v)$ and $\mathrm{dn}(u+v)$. (See Whittaker and Watson [27] and Exercise 11 of Section 1.7.)

Chapter Three

Jacobi's Triple Product and Some Number Theoretic Applications

Abstract. *We establish Jacobi's triple-product identity and apply it quite variously. We first use it to derive the fundamental product identities for the theta functions. We then rederive the triple product via Cauchy's q-binomial theorem and present Bressoud's beautiful elementary proof of the celebrated Rogers–Ramanujan identities. After this we derive Jacobi's formula for $r_4(k)$ (the representation of k as a sum of four squares) and two partition results due to Ramanujan. We also establish the Gaussian sum formula and indicate another proof of the theta transformation formula. Then we briefly discuss the Mellin transform and use it to give the classical reflection formula for the Riemann zeta function. Finally, we show how certain reciprocal series can be evaluated in terms of theta functions. In particular, we give a result due to Landau on the Fibonacci numbers. We also sum the squares of the reciprocals of the Fibonacci numbers.*

3.1 *JACOBI'S TRIPLE-PRODUCT IDENTITY*

Our first proof of the triple-product identity is:

Theorem 3.1

For each pair of complex numbers x and q, with $x \neq 0$ and $|q|<1$,

$$\prod_{n=1}^{\infty}(1+xq^{2n-1})(1+x^{-1}q^{2n-1})(1-q^{2n}) = \sum_{n=-\infty}^{\infty} x^n q^{n^2}. \tag{3.1.1}$$

Proof. Let $F(x, q) := \Pi_{n=1}^{\infty}(1+xq^{2n-1})(1+x^{-1}q^{2n-1})$. Now $F(\cdot, q)$ is

analytic except at zero and has a Laurent expansion at zero. Observe that $F(x, q) = F(x^{-1}, q)$ and $F(xq^2, q) = (xq)^{-1}F(x, q)$. Thus if

$$F(x, q) = \sum_{n=-\infty}^{\infty} c_n(q)x^n$$

then $c_n(q) = c_{-n}(q)$ and $c_n(q) = q^{2n-1}c_{n-1}(q)$ for $n \geq 0$. It follows that $c_n(q) = q^{n^2}c_0(q)$ and

$$F(x, q) = c_0(q) \sum_{n=-\infty}^{\infty} x^n q^{n^2}. \tag{3.1.2}$$

It remains to evaluate $c_0(q)$. Letting $x := 1$ in (3.1.2) gives $c_0(q)\theta_3(q) = \Pi_{n=1}^{\infty}(1+q^{2n-1})^2$ and letting $x := -1$ gives $c_0(q)\theta_4(q) = \Pi_{n=1}^{\infty}(1-q^{2n-1})^2$. Since $\sqrt{\theta_3(q)\theta_4(q)} = \theta_4(q^2)$, we deduce that

$$c_0(q)\theta_4(q^2) = \prod_{n=1}^{\infty}(1-q^{4n-2}).$$

But on replacing q by q^2,

$$c_0(q^2)\theta_4(q^2) = \prod_{n=1}^{\infty}(1-q^{4n-2})^2.$$

Hence

$$\frac{c_0(q^2)}{c_0(q)} = \prod_{n=1}^{\infty}[1-(q^2)^{2n-1}].$$

Since $c_0(0) = 1$ and c_0 is analytic at zero,

$$c_0(q)^{-1} = \prod_{k=1}^{\infty}\left[\frac{c_0(q^{2^k})}{c_0(q^{2^{k-1}})}\right] = \prod_{k=1}^{\infty}\prod_{n=1}^{\infty}[1-q^{2^k(2n-1)}]$$
$$= \prod_{m=1}^{\infty}(1-q^{2m}).$$

This establishes (3.1.1). □

It is convenient to make the following notational abbreviations.

$$Q_0 := \prod_{n=1}^{\infty}(1-q^{2n}) \qquad Q_1 := \prod_{n=1}^{\infty}(1+q^{2n})$$
$$Q_2 := \prod_{n=1}^{\infty}(1+q^{2n-1}) \qquad Q_3 := \prod_{n=1}^{\infty}(1-q^{2n-1}). \tag{3.1.3}$$

From these definitions one easily verifies Euler's identity $Q_1Q_2Q_3 = 1$, which may also be written

$$(3.1.4) \qquad \prod_{n=1}^{\infty}(1+q^n)\prod_{n=1}^{\infty}(1-q^{2n-1}) = 1\,.$$

Also

$$(3.1.5i) \qquad Q_0Q_1 = Q_0(q^2)$$
$$(3.1.5ii) \qquad Q_0Q_3 = Q_0(q^{1/2})$$
$$(3.1.5iii) \qquad Q_2Q_3 = Q_3(q^2)$$
$$(3.1.5iv) \qquad Q_1Q_2 = Q_1(q^{1/2})\,.$$

We gather the first three specializations of the triple-product identity into:

Corollary 3.1

For $|q|<1$, one has

$$(3.1.6) \qquad \theta_3(q) = Q_0Q_2^2 = \prod_{n=1}^{\infty}(1-q^{2n})(1+q^{2n-1})^2$$

$$(3.1.7) \qquad \theta_4(q) = Q_0Q_3^2 = \prod_{n=1}^{\infty}(1-q^{2n})(1-q^{2n-1})^2$$

$$(3.1.8) \qquad \theta_2(q) = 2q^{1/4}Q_0Q_1^2 = 2q^{1/4}\prod_{n=1}^{\infty}(1-q^{2n})(1+q^{2n})^2\,.$$

Proof. These follow on using $x := 1$, -1, and q, respectively, in (3.1.1) (Exercise 2). □

More generally, let k and l be real numbers, and let $q := q^k$ and $x := \pm q^l$ in (3.1.1). Then

$$(3.1.9) \qquad \prod_{n=0}^{\infty}(1\pm q^{2kn+k-l})(1\pm q^{2kn+k+l})(1-q^{2kn+2k}) = \sum_{n=-\infty}^{\infty}(\pm 1)^n q^{kn^2+ln}\,.$$

When $k := \frac{3}{2}$ and $l := \frac{1}{2}$, this gives

$$(3.1.10) \qquad \prod_{n=1}^{\infty}(1-q^n) = \sum_{n=-\infty}^{\infty}(-1)^n q^{(3n+1)n/2}\,.$$

This is *Euler's pentagonal number theorem*, which he found empirically and which affords a combinatorial interpretation [Exercise 3b)], as most of these identities do.

When $k := l := \frac{1}{2}$, we have

$$(3.1.11) \qquad \prod_{n=1}^{\infty}(1+q^n)(1-q^{2n}) = \frac{1}{2}\sum_{n=-\infty}^{\infty} q^{(n+1)n/2} = \prod_{n=1}^{\infty}\frac{1-q^{2n}}{1-q^{2n-1}}\,.$$

Finally, $k := \frac{5}{2}$ and $l := \frac{3}{2}, \frac{1}{2}$ give two formulae which play a central role in the Rogers–Ramanujan identities (Section 3.4):

$$(3.1.12a) \qquad \prod_{n=0}^{\infty}(1-q^{5n+1})(1-q^{5n+4})(1-q^{5n+5}) = \sum_{n=-\infty}^{\infty}(-1)^n q^{(5n+3)n/2}$$

$$(3.1.12b) \qquad \prod_{n=0}^{\infty}(1-q^{5n+2})(1-q^{5n+3})(1-q^{5n+5}) = \sum_{n=-\infty}^{\infty}(-1)^n q^{(5n+1)n/2}\,.$$

We finish the section with a slightly less immediate corollary of the triple product. If $q := q^{1/2}$ and $x := q^{1/2}w$, then (3.1.1) becomes

$$(3.1.13) \qquad \prod_{n=1}^{\infty}(1-q^n)(1+q^n w)(1+q^n w^{-1}) = \left(\frac{w}{w+1}\right)\sum_{n=-\infty}^{\infty} w^n q^{n(n+1)/2}\,.$$

The right-hand side is

$$\sum_{m=0}^{\infty}\left(\frac{w^m + w^{-m-1}}{1+w^{-1}}\right)q^{m(m+1)/2} = \sum_{m=0}^{\infty} w^{-m}\left(\frac{w^{2m+1}+1}{w+1}\right)q^{m(m+1)/2}\,.$$

If we now let w tend to -1 from above this gives

$$(3.1.14) \qquad \prod_{n=1}^{\infty}(1-q^n)^3 = \sum_{m=0}^{\infty}(-1)^m(2m+1)q^{m(m+1)/2}\,.$$

Thus with (3.1.10),

$$(3.1.15) \qquad \left[\sum_{m=-\infty}^{\infty}(-1)^m q^{(3m+1)m/2}\right]^3 = \sum_{m=0}^{\infty}(-1)^m(2m+1)q^{m(m+1)/2}\,.$$

Comments and Exercises

The proof of (3.1.2) is due to Gauss [1866]. The AGM identity (2.1.7) was also in his possession, but Jacobi, by elliptic function techniques, was the first to publish a proof of the triple-product identity. There are many proofs in the literature. Given the AGM, none perhaps is as simple as the one given here.

1. Verify the identities (3.1.4) and (3.1.5).

2. a) Prove Corollary 3.1.
b) Show that

$$(3.1.16) \qquad \prod_{n=1}^{\infty}(1+q^{2n-1})^8 = \prod_{n=1}^{\infty}(1-q^{2n-1})^8 + 16q\prod_{n=1}^{\infty}(1+q^{2n})^8\,.$$

3. a) Establish (3.1.9), (3.1.10), and (3.1.11).

b) A *pentagonal number* is a number of the form $n(3n \pm 1)/2$. Show that (3.1.10) implies that every nonpentagonal number can be partitioned into an even number of distinct parts as often as into an odd number of distinct parts. Show that for pentagonal numbers there is a surplus or deficit of 1, depending on whether n is odd or even. This was first observed by Legendre in 1830. (See Dickson [71, vol. 2].)

4. Establish (3.1.12) and give an interpretation in terms of partitions. Ewell [81] observes that Euler's pentagonal number formula (3.1.10) allows one to establish Jacobi's triple product, given (3.1.2). Thus one can base the identity on a combinatorial proof of (3.1.10) such as is given in Hardy and Wright [60].

5. Use (3.1.10) to show that $c_0(q^3)\prod_{n=1}^{\infty}(1-q^{6n}) = 1$.

6. A complex analytic approach to Jacobi's triple-product is as follows.

a) Show that (3.1.1) is equivalent to

$$\theta_4(z, q) = \prod_{n=1}^{\infty}[1-2q^{2n-1}\cos 2z + q^{4n-2}]\prod_{n=1}^{\infty}(1-q^{2n}) \tag{3.1.17}$$

where $q := e^{\pi i t}$.

b) From the discussion of Section 2.6 show that both sides of (3.1.17) are analytic with zeros at $z = (n+\frac{1}{2})\pi t + m\pi$ (n, m integral). By Liouville's theorem they differ only by a multiplicative constant.

c) Use Exercise 5 to show that this constant is 1.

7. a) Justify taking the limit in (3.1.14).

b) Prove that (3.1.15) is equivalent to

$$\left[\sum_{n=-\infty}^{\infty}(-1)^n q^{(6n+1)^2}\right]^3 = \sum_{m=0}^{\infty}(-1)^m(2m+1)q^{3(2m+1)^2}. \tag{3.1.18}$$

c) Observe that (3.1.18) has the following number theoretic interpretation due to Catalan (Dickson [71, vol. 2]). The excess in the number of even values of $x+y+z$ in

$$(6x\pm 1)^2 + (6y\pm 1)^2 + (6z\pm 1)^2 = 3(2n+1)^2$$

over the number of odd values of $x+y+z$ is $(2n+1)(-1)^n$. In particular, any number of the form $3(2n+1)^2$ must have at least $(2n+1)/6$ decompositions as a sum of three squares.

8. a) Show that θ_3 and θ_4 never vanish ($|q|<1$).

b) Show that θ_2 and θ_3 increase monotonically on $(0,1)$ and θ_4 decreases monotonically on $(0,1)$.

9. Let $p(n)$ denote the number of *partitions* of a natural number n into positive integral parts (the order being irrelevant). Thus $p(4)=5$ and $p(5)=7$.

a) Show that

$$1+\sum_{n=1}^{\infty}p(n)q^n = \prod_{n=1}^{\infty}(1-q^n)^{-1} = 1+\sum_{n=1}^{\infty}\frac{q^{n^2}}{\prod_{k=1}^{n}(1-q^k)^2}. \tag{3.1.19}$$

For the second equality see also Proposition 3.4 of Section 3.3.

b) Use

$$\left[1+\sum_{n=1}^{\infty}p(n)q^n\right]\sum_{n=-\infty}^{\infty}(-1)^n q^{n(3n+1)/2} = 1$$

to write (and implement) a recursive formula for $p(n)$. This is how MacMahon (1918) computed $p(n)$, $1\le n\le 200$; $p(200) = 3972999029388$. For more information on partition theory the reader is referred to Hardy and Wright [60] or Andrews [76].

c) (*Euler*) Establish that

$$\sum_{m\ \text{even}} p(n-a(m)) = \sum_{m\ \text{odd}} p(n-a(m))$$

where $a(m) := m(3m+1)/2$ is the mth pentagonal number.

3.2 *SOME FURTHER THETA FUNCTION IDENTITIES*

In this section we collect a number of definitions and relations, some of intrinsic interest and some for future reference.

Let $r\in(0,\infty)$ and define $\lambda^*(r) := k(e^{-\pi\sqrt{r}})$. As in Chapter 2, we consider k as a function of q $(=e^{-\pi\sqrt{r}})$. Then

$$0 \le 4e^{-\pi\sqrt{r}/2} - \lambda^*(r) = 16e^{-3\pi\sqrt{r}/2} + O(e^{-5\pi\sqrt{r}/2}) \tag{3.2.1}$$

since $\lambda^*(r) = \theta_2^2(e^{-\pi\sqrt{r}})/\theta_3^2(e^{-\pi\sqrt{r}})$ (See Exercise 1.). Also

$$\frac{K'}{K}[\lambda^*(r)] = \sqrt{r}. \tag{3.2.2}$$

From Corollary 3.1 we have

$$\frac{\theta_2(q)}{\theta_3(q)} = \sqrt{k} = 2q^{1/4}\prod_{n=1}^{\infty}\left(\frac{1+q^{2n}}{1+q^{2n-1}}\right)^2 \tag{3.2.3i}$$

(3.2.3*ii*) $$\frac{\theta_4(q)}{\theta_3(q)} = \sqrt{k'} = \prod_{n=1}^{\infty}\left(\frac{1-q^{2n-1}}{1+q^{2n-1}}\right)^2$$

when $q := e^{-\pi K'(k)/K(k)}$.

We next derive another beautiful identity due to Jacobi, in which θ_1^+ denotes the derivative of θ_1 with respect to z at zero. [See equation (2.6.1).]

Proposition 3.1

For $|q|<1$,

(3.2.4) $$\theta_2(q)\theta_3(q)\theta_4(q) = 2\sum_{n=0}^{\infty}(-1)^n(2n+1)q^{(n+1/2)^2} = \theta_1^+(q).$$

Proof. Identity (3.1.14) can be rewritten as

$$\begin{aligned}\theta_1^+(q) &= 2q^{1/4}Q_0^3 = 2q^{1/4}Q_0^3(Q_1Q_2Q_3)^2\\ &= (2q^{1/4}Q_0Q_1^2)(Q_0Q_2^2)(Q_0Q_3^2) = \theta_2\theta_3\theta_4. \quad \square\end{aligned}$$

For various applications to lattice sums it is natural to augment our theta definitions by

(3.2.5) $$\theta_5(q) := 2\sum_{n=-\infty}^{\infty}(-1)^n q^{(2n-1/2)^2}$$

and

(3.2.6) $$\theta_6^+(q) := 2\sum_{n=0}^{\infty}(-1)^{n(n-1)/2}(2n+1)q^{(n+1/2)^2}.$$

By similar arguments [see (3.1.14)] one can show that

(3.2.7) $$\theta_5(q) = 2q^{1/4}Q_0Q_1/Q_2(q^2) = \sqrt{2}\theta_2^{1/2}(q^2)\theta_4^{1/2}(q^2)$$

and

(3.2.8) $$\theta_6^+(q) = \theta_5\theta_3^2(q^2) = \theta_2\theta_3(q^2)\theta_4(q^4).$$

We leave these identities as Exercise 6 and note that (3.2.4) and (3.2.8) have number theoretic interpretations like that of (3.1.15). These three identities and their remanipulations are among the very few known reductions of three theta terms to one known theta expression. (See Glasser and Zucker [80].)

Following Weber [08] and others, it is usual to identify the following quantities. With q and r as above and $\tau := i\sqrt{r}$,

(3.2.9*i*) $$\eta = \eta(\sqrt{-r}) = \eta(\tau) := q^{1/12}Q_0$$

(3.2.9*ii*) $$f_1 = f_1(\sqrt{-r}) = f_1(\tau) := q^{-1/24}Q_3 = (4k'^2/k)^{1/12}$$

(3.2.9*iii*) $$f_2 = f_2(\sqrt{-r}) = f_2(\tau) := 2^{1/2}q^{1/12}Q_1 = (4k^2/k')^{1/12}$$

(3.2.9*iv*) $$f = f(\sqrt{-r}) = f(\tau) := q^{-1/24}Q_2 = (4/kk')^{1/12}.$$

Then

(3.2.10*i*) $$f_1f_2f = \sqrt{2}$$

(3.2.10*ii*) $$f^8 = f_1^8 + f_2^8$$

and K satisfies

(3.2.11) $$K = \frac{\pi}{2}\eta^2f^4 = \frac{\pi}{2k'}\eta^2f_1^4 = \frac{\pi}{2k}\eta^2f_2^4.$$

As will be discussed in Chapter 4, whenever r is rational, f_1, f_2, and f satisfy algebraic equations (whose degree is determined by the number of quadratic forms with determinant $-4r$). Thus once η and one other of f_1, f_2, f, k, k' is known, all six are determined.

A significant identity which follows from (3.2.9*iv*) is

(3.2.12) $$\sum_{n,m=-\infty}^{\infty}{}' \frac{(-1)^{m+n}}{m^2+rn^2} = \frac{-4\pi}{\sqrt{r}}\log[f(\sqrt{-r})] = \frac{\pi}{3\sqrt{r}}\log\left(\frac{kk'}{4}\right).$$

Here and hereafter, the prime over a summation indicates that the term $m=n=0$ is omitted and summation is over expanding rectangles. One establishes (3.2.12) by writing

$$\begin{aligned}-\frac{2\pi}{\sqrt{r}}\log(Q_2) &= \frac{\pi}{\sqrt{r}}\sum_{k=1}^{\infty}\sum_{n=0}^{\infty}\frac{(-1)^k}{k}2q^{(2n+1)k}\\ &= \pi\sum_{k=1}^{\infty}\frac{(-1)^k}{\sqrt{r}k}\operatorname{cosech}(\pi\sqrt{r}k) = \sum_{k=1}^{\infty}\sum_{m=-\infty}^{\infty}\frac{(-1)^{k+m}}{m^2+rk^2}\end{aligned}$$

[using (2.2.3)], and so

$$\sum_{n,m=\infty}^{\infty}{}' \frac{(-1)^{m+n}}{m^2+rn^2} = -\frac{4\pi}{\sqrt{r}}\log(Q_2) - \frac{\pi^2}{6}$$

since $\Sigma_{m=1}^{\infty}(-1)^{m+1}/m^2 = \pi^2/12$. This is the desired result. One may observe that whenever one can evaluate the double sum, one can also evaluate kk'.

In some future work we will be following Ramanujan rather than Weber. Ramanujan studied

$$G_n := (2kk')^{-1/12} = 2^{-1/4} f(\sqrt{-n}) \tag{3.2.13}$$
$$g_n := \left(\frac{k'^2}{2k}\right)^{1/12} = 2^{-1/4} f_1(\sqrt{-n}) .$$

For some purposes these give slightly cleaner results. For example,

$$G_{25} = \frac{\sqrt{5}+1}{2} \qquad g_{10} = \sqrt{\frac{\sqrt{5}+1}{2}} .$$

For the moment we denote $k(q^n)$ by δ and $K(\delta)$ by Λ. We have

$$kk'\left(\frac{2K}{\pi}\right)^3 = 4\sqrt{q}Q_0^6 \tag{3.2.14}$$

so that

$$\left(\frac{kk'}{\delta\delta'}\right)^{1/6} \sqrt{\frac{K}{\Lambda}} = \frac{q^{1/12}Q_0}{q^{n/12}Q_0(q^n)} . \tag{3.2.15}$$

We also have

$$\left(\frac{2K}{\pi}\right)^2 (1-2k^2) = 1 - 24\sum_{n=0}^{\infty} \frac{(2n+1)q^{2n+1}}{1+q^{2n+1}} \tag{3.2.16}$$

$$\left(\frac{2K}{\pi}\right)^4 (1-k^2k'^2) = 1 + 240\sum_{n=1}^{\infty} \frac{n^3q^{2n}}{1-q^{2n}} \tag{3.2.17}$$

and

$$\left(\frac{2K}{\pi}\right)^6 (1-2k^2)\left(1+\frac{1}{2}k^2k'^2\right) = 1 - 504\sum_{n=1}^{\infty} \frac{n^5q^{2n}}{1-q^{2n}} . \tag{3.2.18}$$

These formulae lie considerably deeper, either in elliptic function theory, or as direct computations. Indeed each formula entails formulae for powers of theta functions. We prove only (3.2.16) and leave (3.2.17) as an exercise. We need an identity whose proof we also leave as an exercise.

Lemma 3.1

For $|q|<1$,

$$\sum_{n=0}^{\infty} \frac{nq^n}{1+q^n} = \sum_{n=0}^{\infty} \frac{(2n+1)q^{2n+1}}{1-q^{2n+1}} . \tag{3.2.19}$$

Proposition 3.2

For $|q|<1$,

$$\theta_3^4(q) = 1 + 8\sum_{n=0}^{\infty} \frac{2nq^{2n}}{1+q^{2n}} + 8\sum_{n=0}^{\infty} \frac{(2n+1)q^{2n+1}}{1-q^{2n+1}} \tag{3.2.20}$$

$$\theta_2^4(q) = 8\sum_{n=0}^{\infty} \frac{(2n+1)q^{2n+1}}{1+q^{2n+1}} + 8\sum_{n=0}^{\infty} \frac{(2n+1)q^{2n+1}}{1-q^{2n+1}} \tag{3.2.21}$$

$$\theta_4^4(q) = 1 + 8\sum_{n=0}^{\infty} \frac{2nq^{2n}}{1+q^{2n}} - 8\sum_{n=0}^{\infty} \frac{(2n+1)q^{2n+1}}{1+q^{2n+1}} . \tag{3.2.22}$$

Proof. From (2.3.16), on differentiating with respect to $q = e^{-\pi s}$, and Corollary 3.1 we have

$$\theta_3^4(q) = -4q\left(\frac{\dot\theta_4}{\theta_4} - \frac{\dot\theta_2}{\theta_2}\right) = 8q\frac{d}{dq}\log\left(\frac{Q_1}{Q_3}\right) + 1$$

which yields (3.2.20). The other two follow similarly. □

Theorem 3.2

For $|q|<1$,

$$\theta_3^4(q) = 1 + 8\sum_{\substack{n\not\equiv 0 \pmod 4\\ n\geq 1}} \frac{nq^n}{1-q^n} \tag{3.2.23}$$

and

$$\theta_4^4(q) - \theta_2^4(q) = 1 - 24\sum_{n=0}^{\infty} \frac{(2n+1)q^{2n+1}}{1+q^{2n+1}} . \tag{3.2.24}$$

Proof. Apply Lemma 3.1 to (3.2.20) to establish (3.2.23). To prove (3.2.24) one uses the lemma with q and $-q$. □

Now (3.2.16) is immediate from (3.2.24). Formula (3.2.17) is similarly derived, if one knows in addition (see Rademacher [73]) that

$$\theta_3^8(-q) = \theta_4^8(q) = 1 + 16\sum_{n=1}^{\infty} \frac{(-1)^n n^3 q^n}{1-q^n} . \tag{3.2.25}$$

Finally, (3.2.18) follows from (see Rademacher [73])

$$\theta_3^{12}(q) = 1 + 8\sum_{n=1}^{\infty} \frac{n^5q^n}{1-q^{2n}} - 8\sum_{n=1}^{\infty} \frac{(-1)^n n^5 q^{2n}}{1-q^{2n}} + (\theta_1^+)^4 \tag{3.2.26}$$

Of course, implicit in (3.2.23) is a formula for the number of representations of n as a sum of four squares. We discuss this more fully later.

Comments and Exercises

1. Establish the asymptotic of (3.2.1).

Proposition 3.1 is often established by analytic arguments like those of Exercise 6 of Section 3.1. Proposition 3.1 may then be used, as it is in Whittaker and Watson, to establish the triple-product identity. (See Exercise 6.)

2. a) Show that

$$\prod_{n=0}^{\infty}[1-e^{-(2n+1)\pi}]=2^{1/8}\,e^{-\pi/24}.$$

b) Show that

$$\sum_{n=0}^{\infty} e^{-(2n+1)^2\pi}=(2^{1/4}-1)\pi^{-3/4}2^{-11/4}\Gamma\left(\frac{1}{4}\right).$$

(This was set in Trinity College, Cambridge, in 1881.)

c) Recall that if $k:=(\sqrt{3}-1)/\sqrt{8}$, then $kk'=\frac{1}{4}$ and $K'(k)=\sqrt{3}K(k)$. Deduce that

$$\prod_{n=1}^{\infty}(1+e^{-2n\pi/\sqrt{3}})=2^{-13/24}(\sqrt{3}+1)^{1/4}e^{\pi/12\sqrt{3}}.$$

d) Similarly, if $k:=\sqrt{2}(3-\sqrt{7})/8$, then $kk'=\frac{1}{16}$ and $K'(k)=\sqrt{7}K(k)$. Deduce that

$$\prod_{n=1}^{\infty}(1+e^{-2n\pi/\sqrt{7}})=2^{-5/8}(3+\sqrt{7})^{1/4}\,e^{\pi/12\sqrt{7}}.$$

3. Establish the identities in (3.2.9), (3.2.10), (3.2.11), (3.2.14), and (3.2.15).

4. a) Justify the derivation and convergence of (3.2.12).
b) Evaluate the left-hand sum when $r:=1, 2, 3, 4, 7$.
c) Prove that as r tends to infinity, the sum converges to $-\pi^2/6$. It is already "close" by the time $r=7$.
d) Prove that

$$\sum_{m=-\infty}^{\infty}\ \sum_{n=-\infty}^{\infty}{}'\ \frac{(-1)^n}{n^2+rm^2}=-\frac{4\pi}{\sqrt{r}}\log[f_1(\sqrt{-r})]=\frac{\pi}{3\sqrt{r}}\log\left(\frac{4k'^2}{k}\right).$$

5. Show that

a) $g_{4n}=2^{1/4}g_nG_n$
b) $G_n=G_{1/n}$ and $g_n^{-1}=g_{4/n}$
c) $(g_nG_n)^8(G_n^8-g_n^8)=\frac{1}{4}$.

6. a) Prove Lemma 3.1 by expanding both sides.
b) Prove (3.2.7) and (3.2.8).
c) Establish Theorem 3.2.
d) Prove (3.2.16) and (3.2.17). Try to prove (3.2.18). Exercise 9 will help.

The next two exercises sketch out some facts about *Jacobi's imaginary quadratic transformations*.

7. a) The transformation $k_1:=k^{-1}$ is given in theta terms by

$$\left(\frac{\theta_3}{\theta_2}\right)^2(e^{-\pi s})=\left(\frac{\theta_4}{\theta_3}\right)^2(e^{-\pi(i+s^{-1})}).$$

b) $K'(k_1)=kK'$ and $K(k_1)=k(K+iK')$.
c) The transformation $k_1:=k'^{-1}$ gives $K'(k_1)=k'K$ and $K(k_1)=k'(K'+iK)$.
d) The transformation $k_1:=ik/k'$ gives $k_1'=-k'^{-1}$, $K(k_1)=k'K$, and $K'(k_1)=k'(K'-iK)$, since $\mathrm{re}(s)>0$.
e) The transformation $k_1=k'/ik$ gives $k_1'=k^{-1}$, $K(k_1)=kK'$, and $K'(k_1)=k(K+iK')$.

8. a) Use $s_1:=i+s^{-1}$ to derive from (2.3.14) that

$$-\frac{1}{2}=s\,\frac{\dot\theta_3(s)}{\theta_3(s)}+s^{-1}\,\frac{\dot\theta_4(s_1)}{\theta_4(s_1)}$$

and

$$-s_1\,\frac{\dot\theta_4(s_1)}{\theta_4(s_1)}=-i\,\frac{\dot\theta_4(s_1)}{\theta_4(s_1)}+s\,\frac{\dot\theta_3(s)}{\theta_3(s)}+\frac{1}{2}.$$

b) Now use Exercise 7a) and (2.3.17) and (2.3.18) to show that when $k_1:=k^{-1}$, $kE(k_1)=E(k)-(k')^2K(k)$.
c) Derive similar formulae for $E(k_1)$ for the other three imaginary transformations.
d) Evaluate K'/K when $k:=\sqrt{6}+\sqrt{2}$.

9. a) For $r:=1, 2, 3, 4$, show that $\theta_3(i^rq)=\theta_3(q^4)+i^r\theta_2(q^4)$.

b) $$\sum_{r=1}^{4} i^{-rj}\theta_3^n(i^rq)=4\sum_{\substack{k=0\\ k\equiv j(\mathrm{mod}\ 4)}}^{n}\binom{n}{k}\theta_3^{n-k}(q^4)\theta_2^k(q^4).$$

c) Evaluate $\theta_3^{4-k}\theta_2^k$ for $k:=1, 2, 3, 4$.

10. Show that

$$\sum_{n=-\infty}^{\infty} \frac{(-1)^n \operatorname{cosech}(3n+1)\pi}{3n+1} = \frac{1}{9}\log[8(2-\sqrt{3})]$$

[Let $r := 9$, $2kk' = (2-\sqrt{3})^2$ in (3.2.12). See (4.6.10).]

The formula for sums of two squares is derived from Jacobi's identity

$$\theta_3^2 = 1 + 4\sum_{n=1}^{\infty} \frac{q^n}{1+q^{2n}}. \tag{3.2.27}$$

This will be shown in Chapter 9.

11. A comprehensive list of hyperbolic identities can be derived, as was (3.2.12). We have, for $q := e^{-\pi s}$,

(3.2.28*i*)
$$-\log Q_0 = \sum_1^{\infty} \frac{1}{n(e^{2\pi ns}-1)} = \frac{1}{2}\sum_1^{\infty} \frac{\coth(\pi ns)-1}{n} = -\frac{\pi s}{12} - \frac{1}{6}\log\left(\frac{2K^3kk'}{\pi^3}\right)$$

(3.2.28*ii*)
$$-\log Q_1 = \sum_1^{\infty} \frac{(-1)^n}{n(e^{2\pi ns}-1)} = \frac{1}{2}\sum_1^{\infty} \frac{(-1)^n[\coth(\pi ns)-1]}{n} = -\frac{\pi s}{12} - \frac{1}{12}\log\left(\frac{k^2}{16k'}\right)$$

(3.2.28*iii*)
$$-\log Q_2 = \frac{1}{2}\sum_1^{\infty} \frac{(-1)^n \operatorname{cosech}(\pi ns)}{n} = \frac{\pi s}{24} - \frac{1}{12}\log\left(\frac{4}{kk'}\right)$$

(3.2.28*iv*)
$$-\log Q_3 = \frac{1}{2}\sum_1^{\infty} \frac{\operatorname{cosech}(\pi ns)}{n} = \frac{\pi s}{24} - \frac{1}{12}\log\left(\frac{4k'^2}{k}\right)$$

(3.2.28*v*)
$$\log Q_0 Q_1^2 = \log \frac{\theta_2}{2q^{1/4}} = \sum_1^{\infty} \frac{1}{n(e^{2\pi ns}+1)} = \frac{1}{2}\sum_1^{\infty} \frac{1-\tanh(\pi ns)}{n} = \frac{\pi s}{4} + \frac{1}{2}\log\left(\frac{kK}{2\pi}\right)$$

(3.2.28*vi*)
$$\frac{1}{2}\log Q_0 Q_2^2 = \frac{1}{2}\log\theta_3 = \sum_1^{\infty} \frac{1}{(2n-1)[e^{\pi(2n-1)s}+1]} = \frac{1}{4}\log\left(\frac{2K}{\pi}\right)$$

(3.2.28*vii*)
$$-\frac{1}{2}\log Q_0 Q_3^2 = -\frac{1}{2}\log\theta_4 = \sum_1^{\infty} \frac{1}{(2n-1)[e^{\pi(2n-1)s}-1]} = \sum_1^{\infty} \tanh^{-1} e^{-\pi ns} = -\frac{1}{4}\log\left(\frac{2k'K}{\pi}\right)$$

(3.2.28*viii*)
$$\log\left[\frac{Q_1(q^2)}{Q_2(q^2)}\right] = \sum_1^{\infty} \frac{(-1)^n}{n(e^{2\pi ns}+1)} = \frac{1}{2}\sum_1^{\infty} \frac{(-1)^n[1-\tanh(\pi ns)]}{n} = \frac{\pi s}{4} + \frac{1}{2}\log\left(\frac{1-k'}{2k}\right)$$

(3.2.28*ix*)
$$\log Q_1 Q_2^2 = \sum_1^{\infty} \frac{\operatorname{cosech}[\pi(2n-1)s]}{2n-1} = -\frac{1}{4}\log k'.$$

These are taken from Zucker [84]. Many more identities follow by differentiation or as below.

12. a) Show that

$$\sum_{n=0}^{\infty} \frac{(-1)^n}{2n+1}\operatorname{sech}\left[\frac{(2n+1)\pi s}{2}\right] = \frac{1}{2}\sin^{-1} k. \tag{3.2.29}$$

Hint: Use (3.2.28*ix*). Then replace q by $q^{1/2}$ so that k' is replaced by $(1-k)/(1+k)$. Then replace q by $-q$ so that k is replaced by ik/k' (as in Exercise 7).

b) Show that

$$\sum_{n=0}^{\infty} \frac{(-1)^n}{2n+1} \operatorname{sech}\left[\frac{(2n+1)\pi\sqrt{p}}{2}\right] = \begin{cases} \pi/8 & p:=1 \\ \pi/24 & p:=3 \\ \frac{1}{2}\sin^{-1}[(3-\sqrt{7})/4\sqrt{2}] & p:=7 \end{cases}.$$

3.3 A COMBINATORIAL APPROACH TO THE TRIPLE IDENTITY

The *Gaussian or q-binomial coefficients* are polynomials defined by

$$\binom{n}{0}_q := \binom{n}{n}_q := 1$$

and by

(3.3.1) $$\binom{n}{m}_q := \frac{(q)_n}{(q)_m(q)_{n-m}} = \frac{\Pi_{s=n-m+1}^{n}(1-q^s)}{\Pi_{s=1}^{m}(1-q^s)}$$

when $0<m<n$. Here $(q)_n$ is defined by

(3.3.2) $$(q)_s := \prod_{m=1}^{\infty} \frac{1-q^m}{1-q^{s+m}}.$$

This allows for any complex value of s, but we will consider only integral values. Thus for n in $\mathbb{N}$, $(q)_n = \Pi_{s=1}^{n}(1-q^s)$ and $(q)_{-n}^{-1} = 0$. For $m<0$ or $m>n$ we either define $\binom{n}{m}_q$ to be zero, or observe that it is implicit in our definition of $(q)_m$ (for integral m). The next proposition gathers up some easy facts.

Proposition 3.3

For $|q|<1$,

(*a*) $\binom{n+1}{m+1}_q = \binom{n}{m+1}_q + q^{n-m}\binom{n}{m}_q$

(*b*) $\lim_{q\to 1}\binom{n}{m}_q = \binom{n}{m}$

(*c*) $\binom{n}{m}_q$ is a polynomial in q.

Cauchy's binomial theorem is, for $n = 1, 2, 3, \ldots,$

(3.3.3) $$\sum_{m=0}^{n} y^m q^{m(m+1)/2}\binom{n}{m}_q = \prod_{k=1}^{n}(1+yq^k).$$

This is easily established inductively by showing that both sides of (3.3.3) agree for $n=1$ and satisfy

(3.3.4) $$F_n(y,q) = F_{n-1}(y,q) + yq^n F_{n-1}(y,q).$$

One can also argue, combinatorially, that the coefficient of $y^s q^t$ on each side gives the number of partitions of t into s distinct parts not exceeding n.

If we now let $y := xq^{-N}$ and $n := 2N$, we obtain, after some manipulation,

(3.3.5) $$\sum_{m=-N}^{N} x^m q^{m(m+1)/2}\binom{2N}{N-m}_q = \prod_{1}^{N}(1+xq^m)(1+x^{-1}q^{m-1})$$

a result also due to Cauchy.

This bears a striking resemblance to the triple product in the form of (3.1.13). Indeed on letting N tend to ∞ one has $\binom{2N}{N-m}_q^{-1}$ tending to $Q(q) := \Pi_{m=1}^{\infty}(1-q^m)$, and we are left with (3.1.13) if we can justify the exchange of limit and summation (Exercise 3). Thus (3.3.5) deserves to be considered as a finite form of the triple product.

The following Eulerian result will also be used in the next section. For notational simplicity the empty product equals 1.

Proposition 3.4

For $k = 1, ,2, \ldots,$

$$\prod_{j=1}^{k}\frac{1}{1-xq^j} = \prod_{j=0}^{k}\frac{x^j q^{j^2}}{(1-xq)\cdots(1-xq^j)}\binom{k}{j}_q.$$

Proof. Inductively one establishes that each side satisfies

$$G_k(x,q) = G_{k-1}(x,q) + \frac{xq^k}{1-xq}G_{k-1}(xq,q).$$

Obviously the result is true for $k=1$. Alternatively one can argue that the coefficient of $x^t q^s$ on each side counts partitions of s into t parts not exceeding k. □

Comments and Exercises

Here and in the next section we follow Bressoud [83].

1. Prove Proposition 3.3 and (3.3.3).

2. Verify (3.3.5).

3. a) Prove that for $|q|<1$,

$$\lim_{N\to\infty}\binom{2N}{N-m}_q = Q^{-1}(q)\,.$$

b) Justify the exchange of limit and summation in (3.3.5) by observing that the terms possess uniform majorants that are summable.

4. a) Prove Proposition 3.4.
b) Deduce that

$$(3.3.6)\qquad \prod_{j=1}^{\infty}\frac{1}{1-xq^j}=\sum_{j=0}^{\infty}\frac{x^jq^{j^2}}{(1-xq)(1-q)\cdots(1-xq^j)(1-q^j)}$$

and compare with (3.1.19).

3.4 *BRESSOUD'S 'EASY PROOF' OF THE ROGERS–RAMANUJAN IDENTITIES*

The Rogers–Ramanujan identities are

$$(3.4.1)\quad 1+\sum_{m=1}^{\infty}\frac{q^{m^2}}{(1-q)(1-q^2)\cdots(1-q^m)}=\prod_{m=0}^{\infty}\frac{1}{(1-q^{5m+1})(1-q^{5m+4})}$$

$$(3.4.2)\quad 1+\sum_{m=1}^{\infty}\frac{q^{m^2+m}}{(1-q)(1-q^2)\cdots(1-q^m)}=\prod_{m=0}^{\infty}\frac{1}{(1-q^{5m+2})(1-q^{5m+3})}\,.$$

They afford a remarkable combinatorial interpretation (Exercise 1). We use equations (3.1.12*a*) and (3.1.12*b*) and the notation of the last section to rewrite the identities as

$$(3.4.3)\qquad \sum_{m=0}^{\infty}\frac{q^{m^2}}{(q)_m}=Q^{-1}(q)\sum_{m=-\infty}^{\infty}(-1)^mq^{(5m^2+m)/2}$$

$$(3.4.4)\qquad \sum_{m=0}^{\infty}\frac{q^{m^2+m}}{(q)_m}=Q^{-1}(q)\sum_{m=-\infty}^{\infty}(-1)^mq^{(5m^2+3m)/2}\,.$$

It is this form that we establish. The key observation is the following.

Lemma 3.2

For n positive and integral and any complex a,

$$(3.4.5)\qquad \sum_m\frac{x^mq^{am^2}}{(q)_{n-m}(q)_{n+m}}=\sum_s\frac{q^{s^2}}{(q)_{n-s}}\sum_m\frac{x^mq^{(a-1)m^2}}{(q)_{s-m}(q)_{s+m}}\,.$$

Proof. Note that the above sums are all finite. Set $k:=n-m$ and $x:=q^{2m}$ in Proposition 3.4. Then multiply each side by $(q)_{2m}^{-1}$. We get

$$(q)_{n+m}^{-1}=\sum_j\frac{q^{j^2+2mj}}{(q)_{j+2m}}\frac{(q)_{n-m}}{(q)_j(q)_{n-m-j}}\,.$$

Make this substitution for $(q)_{n+m}^{-1}$ in the left-hand side of (3.4.5). We have

$$\sum_m\frac{x^mq^{am^2}}{(q)_{n-m}(q)_{n+m}}=\sum_m\frac{x^mq^{am^2}}{(q)_{n-m}}\sum_j\frac{q^{j^2+2mj}(q)_{n-m}}{(q)_{j+2m}(q)_j(q)_{n-m-j}}$$
$$=\sum_{m,j}\frac{q^{(m+j)^2}}{(q)_{n-m-j}}\frac{x^mq^{(a-1)m^2}}{(q)_j(q)_{j+2m}}\,.$$

We now sum over m and $s:=m+j$ and exhibit the right-hand side of (3.4.5). □

The effect of Lemma 3.2 is to reduce the power of q^{m^2} by 1. Repeated use of the lemma results in an expression which can be handled by the finite triple-product. As we will see, the $k=2$ case of the next result contains the desired identities.

Theorem 3.3

Given positive integers k and N, we have

$$\sum_{s_1,\dots,s_k}\frac{q^{s_1^2+s_2^2+\cdots+s_k^2}}{(q)_{N-s_1}(q)_{s_1-s_2}\cdots(q)_{s_{k-1}-s_k}(q)_{2s_k}}\prod_{m=1}^{s_k}(1+xq^m)(1+x^{-1}q^{m-1})$$

(3.4.6)

$$=(q)_{2N}^{-1}\sum_m x^mq^{[(2k+1)m^2+m]/2}\binom{2N}{N-m}_q\,.$$

Proof. Commence with applying the lemma to the right-hand side of (3.4.6). We have

$$(q)_{2N}^{-1}\sum_m x^mq^{[(2k+1)m^2+m]/2}\binom{2N}{N-m}_q=\sum_m\frac{(xq^{1/2})^mq^{(2k+1)m^2/2}}{(q)_{N-m}(q)_{N+m}}$$
$$=\sum_s\frac{q^{s^2}}{(q)_{N-s}}\sum_m\frac{(xq^{1/2})^mq^{(2k-1)m^2/2}}{(q)_{s-m}(q)_{s+m}}\,.$$

We continue by applying the lemma $k-1$ more times and arrive at

$$\sum_{s_1,s_2,\ldots,s_k} \frac{(q)^{s_1^2+s_2^2+\cdots+s_k^2}}{(q)_{N-s_1}(q)_{s_1-s_2}(q)_{s_{k-1}-s_k}} \sum_m \frac{(xq^{1/2})^m q^{m^2/2}}{(q)_{s_k-m}(q)_{s_k+m}}.$$

We use the finite triple-product (3.3.5) to write

$$\sum_m \frac{(xq^{1/2})^m q^{m^2/2}}{(q)_{s_k-m}(q)_{s_k+m}} = (q)_{2s_k}^{-1} \prod_{m=1}^{s_k} (1+xq^m)(1+x^{-1}q^{m-1}).$$

This completes the proof. □

The theorem is applied by specifying k and/or x. When $x:=-1$, we observe that unless $s_k=0$, the products on the left-hand side are zero. Thus

$$\text{(3.4.7)} \qquad \sum_{s_1,s_2,\ldots,s_{k-1}} \frac{q^{s_1^2+s_2^2+\cdots+s_{k-1}^2}}{(q)_{N-s_1}(q)_{s_1-s_2}\cdots(q)_{s_{k-2}-s_{k-1}}(q)_{s_{k-1}}}$$
$$= (q)_{2N}^{-1} \sum_m (-1)^m q^{[(2k+1)m^2+m]/2} \binom{2N}{N-m}_q.$$

If we let N tend to ∞, we arrive at

$$\text{(3.4.8)} \qquad \sum_{s_1,s_2,\ldots,s_{k-1}} \frac{q^{s_1^2+s_2^2+\cdots+s_{k-1}^2}}{(q)_{s_1-s_2}\cdots(q)_{s_{k-2}-s_{k-1}}(q)_{s_{k-1}}}$$
$$= \prod_{n=1}^{\infty} (1-q^n)^{-1} \sum_{m=-\infty}^{\infty} (-1)^m q^{[(2k+1)m^2+m]/2}.$$

For $k:=1$, the left-hand side is 1 and the formula recaptures Euler's pentagonal number theorem. For $k:=2$, (3.4.8) coincides with the first Rogers–Ramanujan identity (3.4.3). The second identity is derived similarly by specifying $x:=-q$ and $k:=2$ (Exercise 3).

Comments and Exercises

The Rogers–Ramanujan identities were discovered by Rogers in 1894 and rediscovered by Ramanujan in 1913 (a letter to Hardy) and Schur in 1917. They have continued to receive a great deal of interest. As recently as 1979 Baxter rediscovered them in a physical context.

Hardy and Wright say "no proof is really easy (and it would perhaps be unreasonable to expect an easy proof)." Bressoud's proof certainly comes close to contradicting this. Much of the early history can be found in Hardy's footnotes to Ramanujan [62].

1. Show that (3.4.1) says that the number of partitions of n into parts with minimal difference 2 is the number of partitions into parts congruent to 1 or 4 modulo 5. Equally, (3.4.2) says that the number of partitions of n into parts with minimal difference 2 and minimal part 2 is the number of partitions into parts congruent to 2 or 3 modulo 5.
2. Verify the equivalence of (3.4.1) to (3.4.3) and (3.4.2) to (3.4.4).
3. Derive the second identity (3.4.4) from Theorem 3.3. There is an interesting continued fraction associated with the identities.

$$\text{(3.4.9)} \qquad \prod_{n=0}^{\infty} \frac{(1-x^{5n+2})(1-x^{5n+3})}{(1-x^{5n+1})(1-x^{5n+4})} = \frac{\sum_{n=-\infty}^{\infty}(-1)^n x^{(5n+1)n/2}}{\sum_{n=-\infty}^{\infty}(-1)^n x^{(5n+3)n/2}}$$
$$= 1 + \frac{x}{1+}\,\frac{x^2}{1+}\,\frac{x^3}{1+}\cdots.$$

When $x:=e^{-\pi\sqrt{n}}$ (n rational), this is in principle evaluable in closed form. Ramanujan gives

$$\text{(3.4.10)} \qquad 1+\frac{e^{-\pi 2}}{1+}\,\frac{e^{-2\pi 2}}{1+\cdots} = \left[e^{\pi 2/5}\left(\sqrt{\frac{5+\sqrt{5}}{2}} - \frac{\sqrt{5}+1}{2}\right)\right]^{-1}.$$

In a recent paper, Bhargava and Chandrashekar Adiga [84] detail (3.4.9) and other continued fraction identities. The closed form (3.4.10) and its extensions are elaborated on in Ramanathan [84].

4. Investigate the analogue of Theorem 3.3 in which $2k$ replaces $2k+1$.

3.5 *SOME NUMBER THEORETIC APPLICATIONS*

Our first application is a proof of Jacobi's formula for $r_4(n)$, the number of representations of n as a sum of four squares [including sign and permutation so $r_4(2)=24$ and $r_4(1)=8$]

Theorem 3.4

For each positive integer n,

$$\text{(3.5.1)} \qquad r_4(n) = 8 \sum_{\substack{d\mid n \\ d\not\equiv 0 \pmod 4}} d.$$

In particular every positive integer is the sum of four or fewer squares.

Proof. Expand the right-hand side of formula (3.2.23) for $\theta_3^4(q)$ to obtain

$$\theta_3^4(q) = 1 + 8 \sum_{\substack{m=0 \\ 4 \nmid m}}^{\infty} \sum_{k=1}^{\infty} m q^{mk} = 1 + 8 \sum_{n=1}^{\infty} \Bigg(\sum_{\substack{d|n \\ 4 \nmid d}} d \Bigg) q^n .$$

Now compare coefficients with $\theta_3^4(q)$ written as

$$\theta_3^4 = \sum_{n_i=-\infty}^{+\infty} q^{n_1^2+n_2^2+n_3^2+n_4^2} = 1 + \sum_{n=1}^{\infty} r_4(n) q^n . \quad \square$$

The subsidiary conclusion is Lagrange's famous result. Our second application is an analytic proof of Fermat's theorem that any prime of the form $4k+1$ is the sum of two squares. It is convenient to define

$$\sigma_1(n) := \sum_{d|n} d$$

and

(3.5.2) $$w(n) := \sigma_1(n) + \sigma_1(\text{odd } n)$$

where odd(n) is the odd part of n (that is, the largest odd divisor of n). We set $w(n) := 0$ for $n \le 0$. The proof of the following lemma is left as Exercise 3.

Lemma 3.3

The value $w(n)$ is divisible by 4 unless n is an odd square.

Theorem 3.5

An odd prime p is the sum of two integral squares if and only if it is congruent to 1 modulo 4.

Proof. The 'only if' is immediate on consideration of residues mod 4. Now argue as in Proposition 3.2 and Theorem 3.4 to show that

$$q \frac{\dot\theta_4(q)}{\theta_4(q)} = q \frac{d}{dq} \log(Q_0 Q_3^2) = q \frac{d}{dq} (\log Q_3) + q \frac{d}{dq} \log(Q_0 Q_3)$$

$$= -\sum_{n=0}^{\infty} \frac{(2n+1) q^{2n+1}}{1 - q^{2n+1}} - \sum_{n=1}^{\infty} \frac{n q^n}{1 - q^n}$$

(since $Q_0 Q_3 = Q$). Hence, on expanding these expressions (as in Exercise 12 of Section 3.7)

$$-q \frac{\dot\theta_4(q)}{\theta_4(q)} = \sum_{n=1}^{\infty} w(n) q^n .$$

On multiplying by θ_4 and comparing terms we have

(3.5.3) $$w(n) = 2 \sum_{j \ge 1} (-1)^j w(n - j^2) = \begin{cases} 2(-1)^{r+1} r^2 & n = r^2 \\ 0 & \text{otherwise} \end{cases} .$$

Suppose now that $n = p = 4m+1$ with p prime. Then $w(p) = 2\sigma_1(p) = 8m+4$ and we see that

$$4m + 2 + \sum_{j \ge 1} (-1)^j w(p - j^2) = 0 .$$

Thus some $w(p - j^2)$ is not divisible by 4 and Lemma 3.3 implies that $p = j^2 + k^2$ for some integers j and k. $\square$

Our third application is to establish the following reciprocity result for Gaussian sums. Let

$$S(p, q) := \sum_{r=0}^{q-1} e^{-\pi i r^2 p / q}$$

where p and q are nonzero integers.

Theorem 3.6

For positive integers p and q with pq even,

$$S(p, q) = \sqrt{\frac{q}{p}} \frac{1-i}{\sqrt{2}} \overline{S(q, p)} .$$

(Here the bar represents complex conjugation.)

We will prove the result from the transformation formula for θ_3 (2.3.1). This needs the following:

Lemma 3.4

For pq even and q positive,

$$\lim_{\varepsilon \to 0^+} \sqrt{\varepsilon}\, \theta_3\Big(\varepsilon + \frac{ip}{q}\Big) = \frac{1}{q} S(p, q) .$$

Proof. Write $\theta_3(\varepsilon + ip/q) := \Sigma_{n=-\infty}^{\infty} e^{-\pi n^2 (\varepsilon + ip/q)}$. Then

$$\theta_3\Big(\varepsilon + \frac{ip}{q}\Big) = 1 + 2 \sum_{r=1}^{q} e^{-\pi i r^2 p / q} \Bigg[\sum_{s=0}^{\infty} e^{-(r+sq)^2 \varepsilon \pi} \Bigg]$$

on taking the periodicity of $e^{-n^2 \pi i p / q}$ into account. (Here we have used $e^{-\pi i q^2 p / q} = 1$, which entails pq even.) Thus

$$\sqrt{\varepsilon}\,\theta_3\left(\varepsilon+\frac{ip}{q}\right)=\sum_{r=1}^{q}e^{-\pi i r^2 p/q}\left[2\sqrt{\varepsilon}\int_0^\infty e^{-(r+sq)^2\varepsilon\pi}\,ds\right]+O(\sqrt{\varepsilon})$$

on using the integral test. We now take the limit as $\varepsilon\to 0^+$ and calculate that

$$\lim_{\varepsilon\to 0^+}\sqrt{\varepsilon}\int_0^\infty e^{-(r+sq)^2\varepsilon\pi}\,ds=\lim_{\varepsilon\to 0^+}\sqrt{\varepsilon}\int_{r/q}^\infty e^{-\varepsilon\pi q^2 s^2}\,ds$$

$$=\lim_{\varepsilon\to 0^+}\sqrt{\varepsilon}\int_0^\infty e^{-\varepsilon\pi q^2 s^2}\,ds=\frac{1}{\sqrt{\pi}q}\int_0^\infty e^{-t^2}\,dt=\frac{1}{2q}\,.$$

Since $S(p,q)=\Sigma_{r=1}^{q}e^{-\pi i r^2 p/q}$, this gives the desired result. □

Proof of theorem. We now use the theta transform (2.3.1) to write

$$\sqrt{\varepsilon}\,\theta_3\left(\varepsilon+\frac{ip}{q}\right)=\sqrt{\varepsilon}\left(\varepsilon+\frac{ip}{q}\right)^{-1/2}\theta_3\left(\varepsilon\frac{q^2}{p^2}-\frac{iq}{p}+O(\varepsilon^2)\right).$$

Thus the lemma shows that

$$\frac{1}{\sqrt{q}}S(p,q)=e^{-i\pi/4}\frac{q}{\sqrt{p}}\lim_{\varepsilon\to 0^+}\sqrt{\varepsilon}\,\theta_3\left(\varepsilon\frac{q^2}{p^2}-\frac{iq}{p}+O(\varepsilon^2)\right)$$

$$=e^{-i\pi/4}\sqrt{p}\lim_{\varepsilon'\to 0^+}\sqrt{\varepsilon'}\,\theta_3\left(\varepsilon'-\frac{iq}{p}+O(\varepsilon'^2)\right).$$

By Lemma 3.4 applied to $-q$ and p we deduce that

$$\frac{1}{\sqrt{q}}S(p,q)=e^{-i\pi/4}\frac{1}{\sqrt{p}}S(-q,p)\,. \quad □ \tag{3.5.4}$$

Our final application is a partition result of Ramanujan's which relies on the triple-product identity. (See Exercise 9 of Section 3.1 for the definition of p.)

Theorem 3.7

(*a*) $p(5n+4)$ is divisible by 5.
(*b*) $p(7n+5)$ is divisible by 7.

Proof. With $Q(q)=\Pi_{n=1}^{\infty}(1-q^n)$ as before, we write

$$qQ^4(q)=qQ(q)Q^3(q)=\sum_{m=0}^{\infty}\sum_{n=-\infty}^{\infty}(1--1)^{n+m}(2m+1)q^k$$

where $k:=1+(3n+1)n/2+m(m+1)/2$. This uses the triple-product identities (3.1.10) and (3.1.14) multiplied together. One now considers when k is

divisible by 5. Since $2(n+1)^2+(2m+1)^2\equiv 8k(\text{mod }5)$, we must have $2(n+1)^2+(2m+1)^2$ divisible by 5. An inspection of residues shows that this can only happen if $2(n+1)^2$ and $(2m+1)^2$ are both divisible by 5. Hence, $2m+1$ is divisible by 5 and so is the coefficient of q^{5m+5} in $qQ^4(q)$. From the binomial theorem one deduces that

$$(1-q)^{-5}\equiv(1-q^5)^{-1}(\text{mod }5) \tag{3.5.5}$$

in the sense that all coefficients are congruent. It then follows that $Q(q^5)/Q^5(q)\equiv 1(\text{mod }5)$, and hence the coefficient of q^{5m+5} in

$$\frac{qQ(q^5)}{Q(q)}=\frac{qQ^4(q)Q(q^5)}{Q^5(q)}$$

is divisible by 5. But

$$qQ^{-1}(q)=q\frac{Q(q^5)}{Q(q)}Q^{-1}(q^5)$$

$$=\frac{qQ(q^5)}{Q(q)}\prod_{m=1}^{\infty}\left(\sum_{n=0}^{\infty}q^{5mn}\right)$$

so that the coefficient of q^{5m+5} in $qQ^{-1}(q)$ is divisible by 5. However, by Exercise 9 of Section 3.1,

$$qQ^{-1}(q)=q+\sum_{n=2}^{\infty}p(n-1)q^n\,.$$

Case (*b*) is similar, but uses the square of (3.1.14) instead of the product with Euler's series. (See Exercise 5.) □

Comments and Exercises

The identity (3.5.1) was discovered by Jacobi on April 24th, 1828. He also subsequently observed similar number theoretic interpretations of the formulae for θ_2^4 and θ_4^4, and he gave an arithmetic proof of his theorem. The identities can also be found in Gauss's unpublished work. A wealth of this and similar information can be found in Dickson [71, vol. 2].

An analysis of the components of our proof of (3.5.1) shows that it is rather simpler than that in Hardy and Wright [60], which proceeds from $r_2(n)$, or in Rademacher [73], which uses elliptic function arguments. We use only the triple-product identify and the AGM.

1. Show that $r_4(n)$ is 8 times the sum of the odd divisors when n is odd, and $r_4(n)$ is 24 times the sum of the odd divisors when n is even.
2. Show that

$$\left[\sum_{n=0}^{\infty} q^{(2n+1)^2}\right]^4 = \sum_{n=0}^{\infty} \frac{(2n+1)q^{4(2n+1)}}{1-q^{8(2n+1)}}$$

and deduce that the number of representations of n as a sum of 4 odd squares is $16 \sum_{\substack{4dd'=n \\ d,d' \text{ odd}}} d$.

The argument of Theorem 3.5 is due to Ewell [83]. We give the general formula for $r_2(n)$ in Chapter 9.

3. Prove Lemma 3.3. Consider odd and even cases and use the multiplicativity of σ_1.

Gaussian sums arise naturally in the study of cyclotomic polynomials and hence occurred to Gauss while studying constructible polygons. Apparently this led Gauss to the lemniscate and thence to elliptic functions. The formula (3.5.4) (with $p := 2$) plays a key role in establishing the class number formula for binary forms. Landau [58] is sufficiently taken by the result that he presents three proofs. The result we give is due to Dirichlet. The case with $p := 2$ is due to Gauss save for the "detail" of determining the sign of the complex square root. (See Landau for the significance of the sign.) Our proof follows Bellman [61].

4. Show Gauss's result. For $q \ge 1$,

$$\sum_{r=0}^{q-1} e^{-2\pi i r^2/q} = \sqrt{q}\,\frac{1+i^q}{1+i}\,.$$

This, generalized, leads quickly to a proof of quadratic reciprocity. (See Apostol [76*a*].)

There is a host of more recondite modular results on partitions. (See Andrews [76] or Hardy and Wright [60].) The rule of thumb that additive number theory is generally harder than multiplicative theory is born out by the relative paucity of partition information.

5. a) Show that $(1-q)^{-p} \equiv (1-q^p)^{-1} \pmod p$ holds for any prime p.
b) Prove Theorem 3.7(*b*).

There is a combinatorial proof of the theta transformation formula which is suggestive of the arguments used in the sections on the Rogers–Ramanujan identities, in that it produces a 'finite theta transform' and moves to the limit. The proof is due to Polya. Again we follow Bellman [61].

6. a) $(z^{1/2}+z^{-1/2})^{2m} = \sum_{k=-m}^{m} \binom{2m}{m+k} z^k$ for any z and integral m.

b) Let $w := e^{2\pi i/l}$, l a positive integer. Then

$$\sum_{-l/2 \le k \le l/2} [(w^k z)^{1/2} + (w^k z)^{-1/2}]^{2m} = l \sum_{k=-\lfloor m/l \rfloor}^{\lfloor m/l \rfloor} \binom{2m}{m+lk} z^{lk}\,.$$

(Here $\lfloor x \rfloor$ is the greatest integer less than or equal to x.)

c) Fix s and t with t real and positive. Let $l := \lfloor (mt)^{1/2} \rfloor$ and $z = e^{s/l}$. Then

$$\sum_{-l/2 \le k \le l/2} \left\{\frac{e^{(s+2\pi i k)/2l} + e^{-(s+2\pi i k)/2l}}{2}\right\}^{2m}$$

$$= \sum_{-l/2 \le k \le l/2} \left\{1 + \frac{(s+2\pi i k)^2}{8l^2} + \cdots\right\}^{8l^2(m/4l^2)}$$

$$= \sum_{k=-\lfloor m/l \rfloor}^{\lfloor m/l \rfloor} 2^{-2m} l \binom{2m}{m+kl} e^{sk}\,.$$

d) Now let l go to infinity and use

i) $\lim_{n\to\infty}\left(1+\frac{x_n}{n}\right)^n = e^x$ if $\lim_{x\to\infty} x_n = x$

ii) $\lim_{n\to\infty} \frac{n^{1/2}}{4^n}\binom{2n}{n+r_n} = \frac{e^{-x^2}}{\sqrt{\pi}}$ if $\lim_{n\to\infty} \frac{r_n}{\sqrt{n}} = x$.

e) Deduce from c) and d) the following form of the general theta transformation:

$$\sum_{k=-\infty}^{\infty} e^{(s+2\pi i k)^2/4t} = \sqrt{\frac{t}{\pi}} \sum_{k=-\infty}^{\infty} e^{-tk^2+sk}\,.$$

3.6 *THE MELLIN TRANSFORM AND THE ZETA FUNCTION*

We continue our tour through theta function theory with a discussion of the Riemann zeta function. This also allows us to catalogue a few useful properties of the Mellin transform for future use.

The Mellin transform is a specialized Laplace transform defined by

$$M(f) := M_s(f) := \int_0^\infty f(x)x^{s-1}\,dx\,. \tag{3.6.1}$$

For integrable functions with suitable behaviour at zero and infinity, M_s is analytic in a strip $a < \operatorname{re}(s) < b$. For example, the *gamma* function, $\Gamma(s) := \int_0^\infty e^{-x}x^{s-1}\,dx$, is analytic in $\operatorname{re}(s) > 0$. A most useful identity is

$$\int_0^\infty f(xy)x^{s-1}\,dx = y^{-s}\int_0^\infty f(x)x^{s-1}\,dx \qquad y > 0\,. \tag{3.6.2}$$

Under mild conditions, the Mellin transform is invertible and one can identify two functions whose transforms agree for $\mathrm{re}(s) > 0$. (Certainly this is true if the functions are transformable and continuous.) This is an appropriate place to state the following functional characterization of the gamma function, whose proof is left as a guided exercise.

Theorem 3.8

The gamma function is the unique function $f: (0, \infty) \to [0, \infty)$ such that

(*1*) $f(1) = 1$
(*2*) $f(x+1) = xf(x)$ for $x > 0$, and
(*3*) $\log f(x)$ is convex.

Many otherwise tedious facts are easy consequence of this functional characterization of the gamma function. We list three whose proofs are left as exercises. These are the functional relation $\Gamma(s)\Gamma(1-s) = \pi/\sin \pi s$ (1.6.6), the beta function formula $\beta(s, t) = \Gamma(s)\Gamma(t)/\Gamma(s+t)$ (1.6.7), and the *duplication formula*

$$\Gamma(2s) = \pi^{-1/2} 2^{2s-1} \Gamma(s)\Gamma(s + \tfrac{1}{2}) . \tag{3.6.3}$$

We now derive the functional equation for the *Riemann zeta function* $\zeta(s) := \sum_{n=1}^{\infty} n^{-s}$, $\mathrm{re}(s) > 1$. We observe in passing that ζ has an immediate analytic continuation to $\mathrm{re}(s) > 0$ simply by writing

$$\sum_{n=1}^{\infty} (-1)^n n^{-s} + \sum_{n=1}^{\infty} n^{-s} = 2^{1-s} \sum_{n=1}^{\infty} n^{-s}$$

so that

$$\zeta(s) = \frac{1}{1 - 2^{1-s}} \sum_{n=1}^{\infty} (-1)^{n+1} n^{-s} \qquad \mathrm{re}(s) > 0 . \tag{3.6.4}$$

More interestingly, consider $g(t) := [\theta_3(t) - 1]/2$. For $\mathrm{re}(s) > \frac{1}{2}$ we have

$$M_s(g) = \sum_{n=1}^{\infty} n^{-2s} \pi^{-s} \int_0^{\infty} e^{-t} t^{s-1}\, dt = \frac{\Gamma(s)}{\pi^s} \zeta(2s) .$$

Thus

$$\begin{aligned} \Gamma\left(\frac{s}{2}\right) \zeta(s) \pi^{-s/2} &= \int_0^{\infty} t^{s/2-1} g(t)\, dt \\ &= \int_1^{\infty} t^{s/2-1} g(t)\, dt + \int_0^1 t^{-1/2} g\left(\frac{1}{t}\right) t^{s/2-1}\, dt \\ &\quad + \frac{1}{2} \int_0^1 (t^{-1/2} - 1) t^{s/2-1}\, dt . \end{aligned}$$

Here we have used the theta transform for θ_3 (2.3.1) to substitute for g on $[1, \infty)$. This leads to

$$\Gamma\left(\frac{s}{2}\right) \zeta(s) \pi^{-s/2} = -\left(\frac{1}{s} + \frac{1}{1-s}\right) + \int_1^{\infty} \frac{t^{s/2} + t^{(1-s)/2}}{t} g(t)\, dt \tag{3.6.5}$$

if we evaluate the third integral and replace t by $1/t$ in the second integral.

Since $|g(t)| = O(e^{-\pi t})$ as $t \to \infty$, we see that the integral is an entire function of s. Thus $\Gamma(s/2)\zeta(s)$ is analytic except for simple poles at $s = 0, 1$. Since $\Gamma(s)$ has a simple pole at 0, we see that $\zeta(s)$ is analytic except for a simple pole at $s = 1$. In particular (3.6.5) gives an analytic continuation of $\zeta(s)$ to the entire complex plane. Moreover, as Riemann discovered, the right-hand side of (3.6.5) is invariant under the change of variable $s := 1 - s$. Thus we have

$$\Gamma\left(\frac{s}{2}\right) \pi^{-s/2} \zeta(s) = \Gamma\left(\frac{1-s}{2}\right) \pi^{-(1-s)/2} \zeta(1-s) . \tag{3.6.6}$$

This is the celebrated functional equation for the zeta function.

Comments and Exercises

It is also possible to deduce the Poisson summation formula from the functional equation for the zeta function. (See Bellman [61].)

1. a) Use Holder's inequality to show that Γ satisfies theorem 3.8.
b) Conversely, $g(x) := \log f(x)$ satisfies $g(n+1) = \log(n!)$ and

$$x \log n \le g(n+1+x) - g(n+1) \le x \log(n+1) .$$

Thus

$$0 \le g(x) - \log \frac{n!\, n^x}{x(x+1)\cdots(x+n)} \le x \log\left(1 + \frac{1}{n}\right)$$

and

$$\Gamma(x) = \lim_{n\to\infty} \frac{n!\, n^x}{x(x+1)\cdots(x+n)} = f(x) . \tag{3.6.7}$$

This argument is due to Bohr and Mollerup. Interesting extensions can be found in Askey [80] and in Denninger [84].

2. a) Prove formulae (1.6.6), (1.6.7), and (3.6.3). In the latter case write the ostensible identity in the form $\Gamma(x) = f(x)$ and verify that f satisfies Theorem 3.8.
b) Establish that Γ has an analytic continuation to the entire plane with simple poles at the negative integers and zero, and with no zeros.

3. Let

$$f(x) := \int_0^\infty e^{-(t+x^2/4t)}\, t^{-1/2}\, dt.$$

Verify that $f(x)$ and $\sqrt{\pi}\, e^{-x}$ have the same Mellin transforms by using the duplication formula. Hence reprove the result of Exercise 4 of Section 2.2. Alternatively, establish the duplication formula from that exercise.

4. a) Use (3.6.4) and the fact that $\zeta(s)$ has a pole with residue 1 at 1 to show that

$$\sum_{n=1}^{\infty} \frac{(-1)^{n+1}}{n} = \log 2\,.$$

b) Show that $\zeta(-2n) = 0$ for positive integral n. The reflection formula (3.6.6) at least hints of the centrality of the line $\mathrm{re}(s) = \frac{1}{2}$ in the behaviour of the zeta function. The factorization, due to Euler,

$$\zeta(s) = \prod_{p \text{ prime}} (1 - p^{-s})^{-1} \qquad \mathrm{re}(s) > 1$$

shows the connection between prime distribution and the zeta function. The Riemann hypothesis is that all the nontrivial zeros of $\zeta(s)$ lie on $\mathrm{re}(s) = \frac{1}{2}$. The asymptotic distribution of the primes is inextricably tied up with this famous conjecture. (See Rademacher [73].)

5. Use Theorem 3.8 to establish Gauss's multiplication formula,

$$\Gamma(nx) = (2\pi)^{(1-n)/2} n^{nx-1/2} \prod_{k=0}^{n-1} \Gamma\left(x + \frac{k}{n}\right).$$

6. (*Stirling's formula*) The formula is

$$\frac{\Gamma(s+1)}{(s/e)^s \sqrt{2\pi s}} = 1 + o(1) \qquad s \to \infty\,.$$

Outline: Substitute $x = s(1+u)$ in $M_s(e^x)$ and write

$$\Gamma(s+1) = s^{s+1}\, e^{-s} \int_{-1}^{\infty} [(1+u)\, e^{-u}]^s\, du\,.$$

Now replace u by $t\sqrt{2/s}$ and obtain

$$\Gamma(s+1) = s^s\, e^{-s} \sqrt{2s} \int_{-\infty}^{\infty} \psi_s(t)\, dt$$

for a (dominated) kernel $\psi_s(t)$ which approaches e^{-t^2} uniformly for bounded t.

3.7 *EVALUATION OF SUMS OF RECIPROCALS OF FIBONACCI SEQUENCES*

Since the theta functions provide quadratic analogues for the geometric series, it is natural to ask about their relationship to sums of the form

$$\sum_{n=1}^{\infty} a_n^{-1} \qquad \text{where} \qquad a_{n+1} := Ma_n + Na_{n-1} \tag{3.7.1}$$

with a_0 and a_1 given $(M, N \neq 0)$. The one-term $(N = 0)$ recursion leads to the geometric series. The two-term recursion leads to theta series and their relatives. If $\alpha \neq \beta$ are the roots of $x^2 = Mx + N$, then

$$a_n = \frac{(a_1 - \beta a_0)\alpha^n - (a_1 - \alpha a_0)\beta^n}{\alpha - \beta} \tag{3.7.2}$$

(Exercise 1) and

$$\alpha + \beta = M \qquad \alpha\beta = -N\,.$$

We will consider only the case in which $N = \pm 1$ and M is real. We may write $a_{n+1} = (2c)a_n + \varepsilon a_{n-1}$, $|\varepsilon| = 1$, and to assure that α, β are real, we assume $c > \max\{0, -\varepsilon\}$. Then $\alpha\beta = \pm 1$ and

$$\alpha := c + \sqrt{c^2 + \varepsilon} \qquad \beta := c - \sqrt{c^2 + \varepsilon}\,. \tag{3.7.3}$$

We must consider summing series of the form

$$S := \sum_{n=1}^{\infty} \frac{1}{A\alpha^n + B\beta^n}\,. \tag{3.7.4}$$

The following proposition provides the key. We define the *Lambert series*

$$L(\beta) := \sum_{n=1}^{\infty} \frac{\beta^n}{1 - \beta^n} \qquad |\beta| < 1\,. \tag{3.7.5}$$

Proposition 3.5

For $0 < \beta < \alpha$ with $\alpha\beta = 1$,

(*i*) $$\sum_{n=1}^{\infty} \frac{1}{\alpha^n + \beta^n} = \sum_{n=1}^{\infty} \frac{\beta^n}{1 + \beta^{2n}} = \frac{1}{4}\,[\theta_3^2(\beta) - 1]$$

so

(*ii*) $$\sum_{n=1}^{\infty} \frac{1}{\alpha^{2n} + \beta^{2n}} = \sum_{n=1}^{\infty} \frac{\beta^{2n}}{1 + \beta^{4n}} = \frac{1}{4}\,[\theta_3^2(\beta^2) - 1]$$

and

(*iii*) $$\sum_{n=0}^{\infty} \frac{1}{\alpha^{2n+1}+\beta^{2n+1}} = \sum_{n=0}^{\infty} \frac{\beta^{2n+1}}{1+\beta^{4n+2}} = \frac{1}{4}[\theta_3^2(\beta)-\theta_3^2(\beta^2)] = \frac{1}{4}\theta_2^2(\beta^2).$$

Similarly,

(*iv*) $$\sum_{n=1}^{\infty} \frac{1}{\alpha^n-\beta^n} = \sum_{n=1}^{\infty} \frac{\beta^n}{1-\beta^{2n}} = L(\beta)-L(\beta^2)$$

so

(*v*) $$\sum_{n=1}^{\infty} \frac{1}{\alpha^{2n}-\beta^{2n}} = \sum_{n=1}^{\infty} \frac{\beta^{2n}}{1-\beta^{4n}} = L(\beta^2)-L(\beta^4)$$

and

(*vi*) $$\sum_{n=0}^{\infty} \frac{1}{\alpha^{2n+1}-\beta^{2n+1}} = \sum_{n=0}^{\infty} \frac{\beta^{2n+1}}{1-\beta^{4n+2}} = L(\beta)-2L(\beta^2)+L(\beta^4).$$

Proof. (*i*) The first equality follows on multiplying top and bottom by β^n and the second now follows from (3.2.27), the formula for θ_3^2. (*ii*) Now observe that α^2 and β^2 satisfy the hypotheses of (*i*). Then (*iii*) follows on subtraction. We leave (*iv*), (*v*), and (*vi*) as Exercise 2. □

Proposition 3.5 will allow us to sum $\sum_{n=1}^{\infty} a_n^{-1}$ for certain starting values. Specifically, we can handle $\varepsilon = \pm 1$ and $A = \pm B$ in (3.7.3) and (3.7.4).

CASE 1 $(A = -B)$ Let $a_0 := 0$ and $a_1 := 1$. [This normalization comes by setting $A := (2\sqrt{c^2+\varepsilon})^{-1}$.]

(i) $(\varepsilon = -1)$ Then $\alpha\beta = 1$ and $c > 1$. Now

(3.7.6) $$\sum_{n=1}^{\infty} a_n^{-1} = 2\sqrt{c^2-1}[L(\beta)-L(\beta^2)]$$

as follows from (3.7.2) and Proposition 3.5 (*iv*). Similarly, one can evaluate

$$\sum_{n=1}^{\infty} a_{2n}^{-1} = 2\sqrt{c^2-1}[L(\beta^2)-L(\beta^4)]$$

and

$$\sum_{n=0}^{\infty} a_{2n+1}^{-1} = 2\sqrt{c^2-1}[L(\beta)-2L(\beta^2)+L(\beta^4)].$$

(ii) $(\varepsilon = 1)$ Then $\alpha\beta = -1$. Now $\beta < 0$ and

$$\sum_{n=1}^{\infty} a_{2n}^{-1} = 2\sqrt{c^2+1}\sum_{n=1}^{\infty} \frac{1}{\alpha^{2n}-\beta^{2n}} = 2\sqrt{c^2+1}[L(\beta^2)-L(\beta^4)]$$

while

(3.7.7) $$\sum_{n=0}^{\infty} a_{2n+1}^{-1} = 2\sqrt{c^2+1}\sum_{n=1}^{\infty} \frac{1}{\alpha^{2n+1}+|\beta|^{2n+1}} = \frac{\sqrt{c^2+1}}{2}[\theta_3^2(|\beta|)-\theta_3^2(\beta^2)].$$

CASE 2 $(A = B)$ Let $a_0 := 1$ and $a_1 := c$. [This normalization comes from setting $A = \frac{1}{2}$.]

(i) $(\varepsilon = -1)$ Then $\alpha\beta = 1$ and $c > 1$. Now

(3.7.8)
$$\sum_{n=1}^{\infty} a_n^{-1} = \frac{\theta_3^2(\beta)-1}{2}$$
$$\sum_{n=1}^{\infty} a_{2n}^{-1} = \frac{\theta_3^2(\beta^2)-1}{2}$$
$$\sum_{n=0}^{\infty} a_{2n+1}^{-1} = \frac{\theta_3^2(\beta)-\theta_3^2(\beta^2)}{2} = \frac{\theta_2^2(\beta^2)}{2}$$
$$\sum_{n=0}^{\infty} (-1)^n a_n^{-1} = \frac{2\theta_3^2(\beta^2)-\theta_3^2(\beta)+1}{2}.$$

(ii) $(\varepsilon = 1)$ Then $\beta < 0$ and $\alpha|\beta| = 1$. It follows that

(3.7.9) $$\sum_{n=1}^{\infty} a_{2n}^{-1} = \frac{\theta_3^2(\beta^2)-1}{2}$$

and

$$\sum_{n=0}^{\infty} a_{2n+1}^{-1} = 2[L(|\beta|)-2L(\beta^2)+L(\beta^4)].$$

In certain cases the theta series involved above are particularly simple to evaluate. For example, in Case 2(i), we have $\beta = c - \sqrt{c^2-1}$. Thus $c = (\beta+\beta^{-1})/2$. If $\beta := 10^{-m}$, the series $\theta_3(\beta)$ and $\theta_3(\beta^2)$ in (3.7.8) can be evaluated entirely by writing down sequences of 1's and 0's. Thus for

$2c = 10^m + 10^{-m}$, the sums in (3.7.8) can be evaluated at the same speed as one can multiply n-digit numbers. (See Chapter 6.) Moreover, since theta functions can be fast computed for any algebraic β, the series are always fast computable. (See Chapter 7 and Exercise 6.) Hence the series of Exercises 3, 4, and 5 are quadratically computable.

Finally, consider (3.7.7) for $c := \sinh(\pi s)$ and with $s > 0$. Then $a_{n+1} := 2\sinh(\pi s)a_n + a_{n-1}$, $a_0 := 0$, $a_1 := 1$, and

$$S(s) := \sum_{n=0}^{\infty} a_{2n+1}^{-1} = \frac{\cosh(\pi s)}{2}\,[\theta_3^2(e^{-\pi s}) - \theta_3^2(e^{-2\pi s})]\,. \tag{3.7.10}$$

If we use Theorem 2.1, we have

$$\sum_{n=0}^{\infty} a_{2n+1}^{-1} = \frac{\cosh(\pi s)}{\pi}\left(\frac{1-k'}{2}\right)K(k) \tag{3.7.11}$$

where

$$k = \frac{\theta_2^2(e^{-\pi s})}{\theta_3^2(e^{-\pi s})}$$

on using

$$K\left(\frac{1-k'}{1+k'}\right) = \left(\frac{1+k'}{2}\right)K(k)\,.$$

For singular values of k (see Section 4.6), this formula becomes particularly pretty. [See Exercise 6b).]

Comments and Exercises

1. a) Show that when $x^2 = Mx + N$ has distinct roots α and β, $a_{n+1} = Ma_n + Na_{n-1}$ is solved by (3.7.2).

b) If $\alpha = \beta$, show that

$$a_n = na_1\alpha^{n-1} - (n-1)a_0\alpha^n\,.$$

2. Establish (*iv*), (*v*), and (*vi*) of Proposition 3.5.

3. a) Use (3.7.7) to show that for the *Fibonacci numbers*

$$\sum_{n=0}^{\infty} F_{2n+1}^{-1} = \frac{\sqrt5}{4}\,\theta_2^2\left(\frac{3-\sqrt5}{2}\right) = \frac{\sqrt5}{4}\left[\theta_3^2\left(\frac{\sqrt5-1}{2}\right) - \theta_3^2\left(\frac{3-\sqrt5}{2}\right)\right].$$

Here $F_0 := 0$, $F_1 := 1$, and $F_{n+1} := F_n + F_{n-1}$. This result is due to Landau [1899], as is

b)
$$\sum_{n=1}^{\infty} F_{2n}^{-1} = \sqrt5\left[L\left(\frac{3-\sqrt5}{2}\right) - L\left(\frac{7-3\sqrt5}{2}\right)\right].$$

This is also discussed in Ribenboim [85].

c) The *Lucas numbers* are defined by the same recurrence, $L_{n+1} := L_n + L_{n-1}$ but with $L_0 := 2$ and $L_1 := 1$. (See Hardy and Wright [60].) Show that

$$\sum_{n=0}^{\infty} L_{2n}^{-1} = \left[\theta_3^2\left(\frac{3-\sqrt5}{2}\right) + 1\right]\Big/4\,.$$

d) Note that $x_n := F_{2n+1}$ satisfies $x_{n+1} := 3x_n - x_{n-1}$, $x_0 := 1$, and $x_1 := 2$. Similarly, $x_n := L_{2n}$ satisfies $x_{n+1} := 3x_n - x_{n-1}$, $x_0 := 2$, and $x_1 := 3$.

4. a) Verify (3.7.8) and (3.7.9).

b) Show that for $a_{n+1} := 4a_n - a_{n-1}$, $a_0 := 1$, $a_1 := 2$, one has

$$\sum_{n=1}^{\infty} a_n^{-1} = \frac{\theta_3^2(2-\sqrt3) - 1}{2}$$

and

$$\sum_{n=0}^{\infty} (-1)^n a_n^{-1} = \frac{2\theta_3^2(7-4\sqrt3) - \theta_3^2(2-\sqrt3) + 1}{2}\,.$$

5. Let $a_0 := 0$, $a_1 := 1$, and $a_{n+1} := 9.9a_n + a_{n-1}$. Show that

$$2\sum_{n=0}^{\infty} a_{2n+1}^{-1} = 5.05\left[\theta_3^2\left(\frac{1}{10}\right) - \theta_3^2\left(\frac{1}{100}\right)\right].$$

6. a) Recall that $\theta_3^2(q) = (2/\pi)K(k)$, where $q = e^{-\pi K'/K(k)}$. As shown in Chapter 7, it is possible to quadratically compute k given q. Since K is quadratically computable given k, we can fast compute $\theta_3(q)$ given q.

b) Show that with $S(s)$ given by (3.7.10), we have

$$S(1) = \frac{\cosh(\pi)}{\pi}\left(\frac{\sqrt2-1}{2\sqrt2}\right)K\left(\frac{1}{\sqrt2}\right)$$

$$S(\sqrt2) = \frac{\cosh(\pi\sqrt2)}{\pi}\left(\frac{1-\sqrt{2\sqrt2-2}}{2}\right)K(\sqrt2-1)$$

$$S(\sqrt3) = \frac{\cosh(\pi\sqrt3)}{\pi}\left(\frac{2-\sqrt{2+\sqrt3}}{4}\right)K\left(\frac{\sqrt2(\sqrt3-1)}{4}\right).$$

c) Show that $S(s) = \cosh(\pi s)\,\Sigma_{n=0}^{\infty} \operatorname{sech}[(2n+1)\pi s]$, so that

$$\sum_{n=0}^{\infty} \operatorname{sech}[(2n+1)\pi s] = \frac{\theta_3^2(e^{-\pi s}) - \theta_3^2(e^{-2\pi s})}{2}$$

and

$$\sum_{n=0}^{\infty} \operatorname{sech}(n\pi s) = \frac{\theta_3^2(e^{-\pi s}) + 1}{2}.$$

d) Show that

$$\sum_{n=0}^{\infty} \pi \operatorname{sech}[(2n+1)\pi] = \frac{(2-\sqrt{2})\Gamma^2(\frac{1}{4})}{16\sqrt{\pi}}.$$

7. Equations (3.2.28) and (3.2.29) can be used to derive closed forms for a host of other reciprocal sums. (F_n and L_n are as in Exercise 3.)

a) Use (3.2.29) to show that

$$\sum_{n=0}^{\infty} \frac{(-1)^n}{(2n+1)F_{2n+1}} = \frac{\sqrt{5}}{4} \arcsin\left[\frac{\theta_2^2(\beta)}{\theta_3^2(\beta)}\right]$$

where $\beta := (3-\sqrt{5})/2$.

b) Use (3.2.28*iv*) to show that

$$\sum_{n=1}^{\infty} \frac{1}{2nF_{2n}} = \frac{\sqrt{5}}{12} \log\left[\frac{\theta_2(\beta^2)\theta_3(\beta^2)}{2\sqrt{\beta}\,\theta_4^2(\beta^2)}\right]$$

where $\beta := (\sqrt{5}-1)/2$.
Use (3.2.28*i*) and transformation formulae to show that

i) $$\sum_{n=1}^{\infty} \operatorname{cosech}^2(n\pi s) = \frac{1}{6} + \frac{2}{\pi^2}\left[\left(\frac{1+k'^2}{3}\right)K^2 - KE\right]$$

ii) $$\sum_{n=1}^{\infty} \operatorname{cosech}^2(2n\pi s) = \frac{1}{6} + \frac{1}{\pi^2}\left[\left(\frac{1+k'^2}{6}\right)K^2 - KE\right]$$

iii) $$\sum_{n=0}^{\infty} \operatorname{cosech}^2[(2n+1)\pi s] = \frac{1}{\pi^2}\left[\left(\frac{1+k'^2}{2}\right)K^2 - KE\right].$$

d) Similarly, use (3.2.28*v*) to show that

i) $$\sum_{n=1}^{\infty} \operatorname{sech}^2(n\pi s) = \frac{2EK}{\pi^2} - \frac{1}{2}$$

ii) $$\sum_{n=1}^{\infty} \operatorname{sech}^2(2n\pi s) = \frac{EK + k'K^2}{\pi^2} - \frac{1}{2}$$

iii) $$\sum_{n=0}^{\infty} \operatorname{sech}^2[(2n+1)\pi s] = \frac{EK - k'K^2}{\pi^2}.$$

e) Show that

i) $$\sum_{n=1}^{\infty} \operatorname{cosech}^2(n\pi) = \frac{1}{6} - \frac{1}{2\pi}$$

ii) $$\sum_{n=0}^{\infty} \operatorname{sech}^2\left[\frac{(2n+1)\pi}{2}\right] = \frac{1}{2\pi}.$$

f) Combine results of c) and d) to show that, with $\beta := (3-\sqrt{5})/2$,

$$\sum_{n=1}^{\infty} F_n^{-2} = \tfrac{5}{24}\,[\theta_2^4(\beta) - \theta_4^4(\beta) + 1] \tag{3.7.12}$$

and

$$\sum_{n=1}^{\infty} L_n^{-2} = \tfrac{1}{8}\,[\theta_3^4(\beta) - 1] \tag{3.7.13}$$

and deduce similar formulae for $\Sigma_{n=1}^{\infty} (-1)^n F_{2n}^{-2}$ and for $\Sigma_{n=1}^{\infty} (-1)^n L_{2n}^{-2}$.

g) Show that the Lucas numbers satisfy

$$\sum_{n=1}^{\infty} L_n^{-2} = 2\left(\sum_{n=1}^{\infty} L_{2n}^{-1}\right)^2 + \sum_{n=1}^{\infty} L_{2n}^{-1}$$

and show that a similar formula holds for all recursions of the form $a_{n+1} = (2c)a_n + a_{n-1}$, $a_0 := 2c$, and $a_1 := 1$.

h) Show that

$$3\sum_{n=1}^{\infty} F_n^{-2} + 5\sum_{n=1}^{\infty} L_n^{-2} = 4\left(\sum_{n=0}^{\infty} F_{2n+1}^{-1}\right)^2.$$

8. a) Show that

$$\sum_{n=1}^{\infty} (-1)^{n+1} \frac{L_{2n}}{F_{2n}^2} = \sum_{n=1}^{\infty} F_n^{-2}.$$

Hint: Differentiate (3.2.28*iii*) and compare the result to Exercise 7f), equation (3.7.12).

b) Show that

$$-2\sum_{m=1}^{\infty}(-1)^m m\,\mathrm{cosech}\,(2m\pi s)=\sum_{m=0}^{\infty}\mathrm{sech}^2\,[(2m+1)\pi s]$$

and hence that

$$\sqrt{5}\sum_{n=1}^{\infty}(-1)^{n+1}\frac{n}{F_{2n}}=\sum_{n=0}^{\infty}F_{2n+1}^{-2}\,.$$

9. Show that

$$\sum_{n=1}^{\infty}\frac{q^n}{[q^n+(-1)^n]^2}=\frac{\theta_3^4(q)-1}{8}$$

$$\sum_{n=1}^{\infty}\frac{(-1)^n q^n}{(q^n+1)^2}=\frac{\theta_4^4(q)-1}{8}$$

and

$$\sum_{n=1}^{\infty}\frac{q^n}{[q^n+(-1)^{n+1}]^2}=\frac{\theta_2^4(q)-\theta_4^4(q)+1}{24}\,.$$

10. a) Show (by expanding both sides) that

$$L(x):=\sum_{n=1}^{\infty}\frac{x^n}{1-x^n}=\sum_{n=1}^{\infty}x^{n^2}\frac{1+x^n}{1-x^n}\,.$$

b) Hence show that all the series considered in this section can be computed with at most $O(\sqrt{n})$ operations for n digits. (See Chapter 6.)

A remarkable elementary result is

$$\sum_{n=0}^{\infty}\frac{1}{F_{2n+1}+F_k}=\frac{k\sqrt{5}}{2F_k}\qquad k=1,3,5\,\ldots.$$

This is a specialization of identities established in Backstrom [81]. (Related results can be found in Carlitz [71].) Thus

$$\sum_{n=0}^{\infty}\frac{1}{F_{2n+1}+1}=\frac{\sqrt{5}}{2}\,.$$

A related formula is

$$\sum_{n=0}^{\infty}\frac{1}{F_{2n+1}+13}=\frac{7\sqrt{5}}{58}\,.$$

11. Show that

$$\sum_{n=0}^{\infty}\frac{1}{L_{2n}+2}=\frac{KE}{2\pi^2}+\frac{1}{8}\qquad(3.7.14)$$

where $q:=(\sqrt{5}-1)/2$. Now k is close to 1, so that $KE/2\pi^2$ is close to

$$\frac{K}{2\pi^2}=\frac{\theta_3^2(q)}{4\pi}=\frac{\theta_3^2[e^{\pi^2/\log[(\sqrt{5}-1)/2]}]}{4\log[(\sqrt{5}+1)/2]}$$

where the last equality follows from the theta transform. One sees that $KE/2\pi^2+\frac{1}{8}$ is close to

$$\frac{1}{4\log[(\sqrt{5}+1)/2]}+\frac{1}{8}$$

which explains, in some part, Backstrom's formal manipulation in Backstrom [81]; and which evaluates (3.7.14) as requested therein. Almqvist [Pr] treats this sum and some relatives. Note that $e^{\pi^2/\log[(\sqrt{5}-1)/2]}\sim 10^{-9}$ so that, as in all these Fibonacci series, transformation considerably speeds convergence.

Lambert series occur naturally in multiplicative number theory, as the following exercise shows.

12. a) Show that for any real valued function f,

$$\sum_{n=1}^{\infty}f(n)\frac{x^n}{1-x^n}=\sum_{n=1}^{\infty}F(n)x^n$$

where

$$F(n):=\sum_{d|n}f(d)\,.$$

This is due to Laguerre. Hence show that

i) $$\sum_{n=1}^{\infty}\frac{x^n}{1-x^n}=\sum_{n=1}^{\infty}\tau(n)x^n$$

where $\tau(n)$ is the number of divisors of n.

ii) $$\sum_{n=1}^{\infty}\frac{n^k x^n}{1-x^n}=\sum_{n=1}^{\infty}\sigma_k(n)x^n\qquad k=1,2,\ldots$$

where $\sigma_k(n)$ is the sum of the kth powers of divisors of n.

b) Let

$$F(n) := \begin{cases} 1 & \text{if } n \text{ is square} \\ 0 & \text{if } n \text{ is nonsquare} \end{cases}.$$

Show that $f(n) = (-1)^{\Sigma e_i}$ where

$$n = \prod_{i=1}^{m} p_i^{e_i} \qquad \text{(in prime decomposition)}.$$

Hint: Use Möbius inversion. Since F is multiplicative, so is f. Thus using Liouville's function $e(n) := (-1)^{\Sigma_{i=1}^{m} e_i}$

$$\sum_{n=1}^{\infty} e(n) \frac{x^n}{1-x^n} = \frac{\theta_3(x) - 1}{2}.$$

c) Show that

$$\sum_{n=1}^{\infty} \frac{e(n)}{F_{2n}} = \frac{\sqrt{5}}{2} [\theta_3(\beta) - \theta_3(\beta^2)]$$

where $\beta := (3 - \sqrt{5})/2$.

Zucker [79] gives general formulae for sums of powers of hyperbolic functions (in which the coefficients are defined recursively and have been computed extensively by Ramanujan and Zucker). Using these one can evaluate $\Sigma_{n=1}^{\infty} (-1)^{n+1} F_n^{-4k}$ and $\Sigma_{n=1}^{\infty} F_n^{-4k+2}$ in terms of θ when $k := 1, 2, 3, \ldots$. There are similar Lucas number results, and if K and E are used, many more sums are expressible. We give two examples:

$$\sum_{n=1}^{\infty} (-1)^{n+1} L_n^{-4} = \frac{1}{96} \{3 + [\theta_2^4(\beta) - 1]^2 - [\theta_4^4(\beta) + 1]^2\}$$

and

$$\sum_{n=0}^{\infty} F_{2n+1}^{-3} = \frac{5\sqrt{5}}{32} \theta_2^2(\beta)[1 - \theta_4^4(\beta)].$$

Here, as before, $\beta := (3 - \sqrt{5})/2$.

13. Let $u_0 := 0$, $u_1 := 1$, and $u_{n+1} := au_n + u_{n-1}$. Let $v_0 := 2$, $v_1 := a$, and $v_{n+1} := av_n + v_{n-1}$.

a) Establish that

$$\sum_{n=1}^{\infty} \frac{(-1)^{n+1}}{\Sigma_{k=1}^{n} u_k^2} = a^2(a^2+4) \sum_{k=1}^{\infty} \frac{1}{v_{4k} + v_2} = \frac{a}{2} (\sqrt{a^2+4} - a).$$

Hint: The second sum in a) can be made to telescope.

b) In particular,

$$\sum_{n=1}^{\infty} \frac{(-1)^{n+1}}{\Sigma_{k=1}^{n} F_k^2} = \frac{\sqrt{5} - 1}{2}.$$

c) Compare

i) $$\sum_{n=1}^{\infty} \frac{(-1)^{n+1}}{\Sigma_{k=1}^{n} k^2} = 6(\pi - 3)$$

and

ii) $$\sum_{n=1}^{\infty} \frac{1}{\Sigma_{k=1}^{n} k^2} = 6(3 - 4\log 2).$$

d) Show that

$$\sum_{n=1}^{\infty} \frac{1}{\Sigma_{k=1}^{n} u_k^2} = \frac{a}{2} (\sqrt{a^2+4} - a) + 2a(a^2+4) \sum_{k=1}^{\infty} \frac{1}{v_{4k+1} - a}$$

$$= \frac{a}{2} (\sqrt{a^2+4} - a) + 2a \sum_{k=1}^{\infty} \frac{1}{u_{2k} u_{2k+1}}.$$

Chapter Four

Higher Order Transformations

Abstract. We develop algebraic transformations of prime order for the elliptic integrals. For small numbers this can be managed purely algebraically. However, the development of modular equations for arbitrary primes is most comfortably effected via transcendental methods. This requires some rudimentary modular function theory. The cubic equation is studied in particular detail.

4.1 A FIRST APPROACH TO HIGHER ORDER TRANSFORMATIONS

The fundamental relation from Theorem 1.2

(4.1.1) $$K(k) = \frac{1}{1+k} K\left(\frac{2\sqrt{k}}{1+k}\right)$$

is remarkable for a number of reasons. One notable consequence is the ab initio unlikely observation that when k is algebraic and

(4.1.2) $$l := \frac{2\sqrt{k}}{1+k}$$

the values of the transcendental function K at l and k are algebraically connected. Equation (4.1.2) is one form of the *quadratic modular equation.* It can be rewritten as

(4.1.3) $$l^2(1+k)^2 - 4k = 0\,.$$

We will develop a class of algebraic equations (modular equations) that induce algebraic transformations on K in a similar fashion.

We commence by sketching, à la Cayley [1895], a purely algebraic

approach to the modular equation. It transpires that this approach becomes unduly complicated for all but a few simple cases and is hard to use as a rigorous basis for the general theory. Thus in Sections 4.3 and 4.4 we will derive the general theory using function theoretic techniques.

We are looking for a relation of the form

(4.1.4) $$\frac{M(l,k)\,dy}{\sqrt{(1-y^2)(1-l^2y^2)}} = \frac{dx}{\sqrt{(1-x^2)(1-k^2x^2)}}$$

where l and k satisfy a polynomial equation Ω in two variables. Such an algebraic connection between the two moduli (l and k) is called a *modular equation* or *modular transformation* for k. Specific but equivalent modular equations for algebraically related functions are defined in (4.4.2), (4.4.6), and (4.5.1). The function M will be an algebraic function of k and l and is called the *multiplier*. With this in mind, let P and Q be polynomials in x^2 so that $\deg(P \pm xQ)^2(1 \pm x) = n$ (n odd) and write

(4.1.5) $$\frac{1-y}{1+y} = \frac{(P-xQ)^2}{(P+xQ)^2}\,\frac{1-x}{1+x}\,.$$

The important condition to impose on P, Q, and $l := l(k)$ is that (4.1.5) must be invariant when (x, y) is replaced by $(1/kx, 1/ly)$. (See Exercise 1.) We now try to solve for P and Q. Set

(4.1.6) $$U := x(P^2 + 2PQ + x^2Q^2) \qquad V := P^2 + 2x^2PQ + x^2Q^2$$
$$A := P - xQ \qquad B := P + xQ$$

and observe that

$$y = U/V$$

(4.1.7*a*) $$1 - y = (1-x)A^2/V \qquad 1 + y = (1+x)B^2/V\,.$$

Also, from the invariance of (4.1.5),

(4.1.7*b*) $$1 - ly = (1-kx)C^2/V \qquad 1 + ly = (1+kx)D^2/V$$

where C and D are polynomials of the same form as P and Q. Thus we deduce that

(4.1.8) $$\frac{dy}{\sqrt{(1-y^2)(1-l^2y^2)}} = \frac{\dot{U}V - \dot{V}U}{ABCD}\,\frac{dx}{\sqrt{(1-x^2)(1-k^2x^2)}}\,.$$

It can now be computed (Exercise 1) that

$$\frac{1}{M(l,k)} = \frac{\dot{U}V - \dot{V}U}{ABCD} = 1 + 2\frac{Q(0)}{P(0)} \tag{4.1.9}$$

is independent of x. Let us return to (4.1.5). For $n = 4p + 1$ we must have

$$\deg P = 2p \qquad \deg Q = 2(p-1)\,. \tag{4.1.10}$$

For $n = 4p + 3$,

$$\deg P = 2p \qquad \deg Q = 2p\,. \tag{4.1.11}$$

Since P and Q are even functions, we have in either case $\frac{1}{2}(n+1)$ degrees of freedom. It remains to use the invariance in (4.1.5) as $(x, y) \to (1/kx, 1/ly)$. This leads immediately to the equation

$$\frac{V(1/kx)}{U(1/kx)} = l\,\frac{U(x)}{V(x)} \tag{4.1.12}$$

since $y = U/V$. Thus we are reduced to solving

$$(P^2 + 2x^2PQ + x^2Q^2)^* = \sqrt{\frac{l}{k}}\,k^{(n-1)/2}(P^2 + 2PQ + x^2Q^2) \tag{4.1.13}$$

where the * operation is defined as follows. If

$$S := a_0 + a_1x + \cdots + a_mx^m$$

then

$$S^* := a_0(kx)^m + a_1(kx)^{m-1} + \cdots + a_m\,.$$

Equating coefficients in (4.1.13) leads to a system of $\frac{1}{2}(n+1)$ nonlinear equations. There are $\frac{1}{2}(n+1)$ degrees of freedom in the coefficients of P and Q. Since the equation is homogeneous in P and Q, one of the coefficients may be assumed to be 1. This leaves one additional condition to be satisfied by k and l and leads to the desired unique algebraic relation between k and l. The pitfalls of this approach are now, of course, apparent. We end up with a large system of nonlinear equations that are virtually impossible to solve or analyse directly.

We illustrate with the cases 3 and 5.

CUBIC TRANSFORMATION $(n = 3)$. We have $P = 1$ and $Q = \alpha$. Equation (4.1.13) becomes

$$k^2x^2 + 2\alpha + \alpha^2 = \sqrt{\frac{l}{k}}\,k(1 + 2\alpha + \alpha^2x^2)\,.$$

This leads to two equations,

$$\begin{aligned} k &= \sqrt{\frac{l}{k}}\,\alpha^2 \\ 2\alpha + \alpha^2 &= \sqrt{\frac{l}{k}}\,k(1+2\alpha)\,. \end{aligned} \tag{4.1.14}$$

This is solved parametrically by

$$k^2 = \frac{\alpha^3(2+\alpha)}{2\alpha+1} \quad \text{and} \quad l^2 = \frac{\alpha(2+\alpha)^3}{(2\alpha+1)^3} \tag{4.1.15a}$$

with similar expressions for $(k')^2$ and $(l')^2$, namely,

$$k'^2 = \frac{(1-\alpha)(1+\alpha)^3}{2\alpha+1} \quad \text{and} \quad l'^2 = \frac{(1+\alpha)(1-\alpha)^3}{(2\alpha+1)^3}\,. \tag{4.1.15b}$$

From this one can deduce that

$$\sqrt{kl} + \sqrt{k'l'} = 1 \tag{4.1.16}$$

or, equivalently,

$$(k^2 - l^2)^4 = 128k^2l^2(1-k^2)(1-l^2)(2 - k^2 - l^2 + 2k^2l^2)\,. \tag{4.1.17}$$

In the associated variables $u := k^{1/4}$ and $v := l^{1/4}$ this has a simpler form, namely,

$$u^4 - v^4 + 2uv(1 - u^2v^2) = 0\,. \tag{4.1.18}$$

(See Section 4.5.) The multiplier M has any of the following forms:

$$M = \frac{1}{2\alpha+1} = \frac{v}{v+2u^3} = \frac{2v^3 - u}{3u}\,. \tag{4.1.19}$$

(See Exercise 2 of this section and Exercise 2 of Section 4.6.)

QUINTIC TRANSFORMATION $(n = 5)$. We have $P = 1 + \beta x^2$ and $Q = \alpha$. Equation (4.1.13) leads to the three equations $(\Delta^2 := k^5/l)$

$$\begin{aligned} \beta^2 &= \Delta \\ k^2(2\alpha\beta + 2\beta + \alpha^2) &= \Delta(2\alpha + 2\beta + \alpha^2) \\ k^4(2\alpha+1) &= \Delta(\beta^2 + 2\alpha\beta)\,. \end{aligned} \tag{4.1.20}$$

This eventually solves, with $u := k^{1/4}$ and $v := l^{1/4}$, as

(4.1.21) $$u^6 - v^6 + 5u^2v^2(u^2 - v^2) + 4uv(1 - u^4v^4) = 0\,.$$

The multiplier M has any of the forms

(4.1.22) $$M = \frac{1}{2\alpha + 1} = \frac{v(1 - uv^3)}{v - u^5} = \frac{u + v^5}{5u(1 + u^3v)}\,.$$

The transformations are called cubic, quintic, and so on, because of the underlying order of the transformation (and so of convergence).

Comments and Exercises

The very classical approach of the section to cubic and quintic modular equations is due to Jacobi [1829]. This algebraic approach was extended to the septic ($n = 7$) case by Cayley [1874], who also treated the endecadic ($n = 11$) case partially. The calculations are formidable. We have followed Cayley closely in this discussion. The associated variables $u := k^{1/4}$ and $v := l^{1/4}$ of Jacobi's considerably simplify the calculations, as we will see in Section 4.5.

In order to find the relationship between $K(l)$ and $K(k)$ implicit in (4.1.4) we must show that the underlying transformation (4.1.5) is one to one and onto on the interval $[0, 1]$. This can be done directly for $n = 3$ (Exercise 3) and other small n. However, as with most of the details, it is easier to use the general transcendental approach of Sections 4.3, 4.4, and 4.5.

1. a) Show that an equation of the form (4.1.5) that is invariant under the change of variables $(x, y) \to (1/kx, 1/ly)$ exists. *Hint*: Set

$$y := \frac{x}{M} \prod_i \frac{1 - x^2/a_i^2}{1 - k^2a_i^2x^2}\,.$$

Replacing (x, y) by $(1/kx, 1/ly)$ gives

$$\frac{1}{ly} = \frac{1}{xMk^n \Pi_i a_i^4} \prod_i \frac{1 - k^2a_i^2x^2}{1 - x^2/a_i^2}$$

which holds, provided that

$$l = M^2k^n\Big(\prod_i a_i\Big)^4\,.$$

[See also (4.1.13).]

b) Establish (4.1.7b) and exhibit C and D.

c) Establish (4.1.9).
Hint: Let U and V be as in (4.1.6). Let $y := U/V$ and let $Y(a, b) := (a^2 - b^2)(a^2 - l^2b^2)$. Then

$$Y(V, U) = (V^2 - U^2)(V^2 - l^2U^2)$$

and

$$\frac{dy}{\sqrt{Y(1, y)}} = \frac{\dot{U}V - U\dot{V}\,dx}{\sqrt{Y(V, U)}}\,.$$

Now observe that any square factor $(x - a)^2$ of $Y(V, U)$ is a linear factor of $V\dot{U} - U\dot{V}$. Since

$$V^2 - U^2 = (1 - x^2)A^2B^2$$

and

$$V^2 - l^2U^2 = (1 - k^2x^2)C^2D^2$$

the fact that $(\dot{U}V - \dot{V}U)/ABCD$ is independent of x now follows. The explicit form of the multiplier $M(l, k)$ is derived by setting $x = 0$ in $(\dot{U}V - \dot{V}U)/ABCD$.

2. a) Establish the four forms of the cubic modular equations (4.1.15), (4.1.16), (4.1.17), and (4.1.18).

b) Complete the calculation of the quintic modular equation (4.1.21).

3. Show that the $n = 3$ relation between x and y underlying the cubic transformation is one to one and onto on $[0, 1]$, and hence (4.1.4) can be integrated over $[0, 1]$.

4. (*An explicit cubic algorithm for* K) The cubic modular equation (4.1.18) is of degree 4 and, hence, can be solved explicitly for u in terms of v.

a) Show, for $v \in (0, 1)$, that $u \in (0, v)$ is a solution of (4.1.18), where

$$u = \frac{v^3}{2} + \frac{D - R}{2}$$

and

$$S := \sqrt[3]{4v^2(1 - v^8)}$$

$$R := \sqrt{v^6 + S}$$

$$D := \sqrt{2v^6 - S + \frac{4v - 2v^9}{R}}\,.$$

b) Show, for $u \in (0, 1)$, that $v \in (u, 1)$ is a solution of (4.1.18), where

$$v = -\frac{u^3}{2} + \frac{D+R}{2}$$

and

$$S := \sqrt[3]{4u^2(1-u^8)}$$

$$R := \sqrt{u^6 + S}$$

$$D := \sqrt{2u^6 - S + \frac{4u - 2u^9}{R}}\,.$$

c) Show, for $v \in (0,1)$, that there is a *unique* $u \in (0, v)$ so that (4.1.18) is solved by (u, v). We can define an iteration as follows. For $v_i \in (0,1)$, let $v_{i+1} \in (0, v_i)$ be such that $u := v_{i+1}$ and $v := v_i$ satisfy the modular equation (4.1.18). Show, using a) and b), that

(4.1.23) $$v_{n+1} = v_n^3 - \sqrt{v_n^6 + \sqrt[3]{4v_n^2(1-v_n^8)}} + v_{n-1}$$

where $v_0 \in (0,1)$ and $v_1 \in (0, v_0)$ is computed from v_0 by Exercise 4a).

d) Show that, for $v_0 \in (0,1)$,

(4.1.24) $$K(v_0^4) = \frac{\pi}{2}\prod_{n=1}^{\infty}\left(1 + \frac{2v_i^3}{v_{i-1}}\right).$$

(Use Exercise 3.)

e) Show that v_i tends to zero cubically. (For further details see Borwein and Borwein [84*b*].)

5. a) Let $u \in (0,1)$ and $v \in (u,1)$ satisfy the cubic modular equation (4.1.18). Show that

(4.1.25) $$\frac{K'(u^4)}{K(u^4)} = 3\,\frac{K'(v^4)}{K(v^4)}\,.$$

Hint:

$$l'^2 = \frac{(1-\alpha)^3(1+\alpha)}{(2\alpha+1)^3} = \frac{(2+\beta)\beta^3}{2\beta+1} \quad \text{if} \quad (2\beta+1)(2\alpha+1) = 3\,.$$

b) Let $u \in (0,1)$ and $v \in (u,1)$ satisfy the quintic modular equation (4.1.21). Show that

(4.1.26) $$\frac{K'(u^4)}{K(u^4)} = 5\,\frac{K'(v^4)}{K(v^4)}\,.$$

Hint: Show that if $(u, v) := (k^{1/4}, l^{1/4})$ satisfies (4.1.21), then so does $(u, v) = (l'^{1/4}, k'^{1/4})$. Now Exercise 1 of Section 1.5 shows that the two sides of the above equation differ by a constant. Use the logarithmic asymptotic at 0 and the relationship between u and v as $v \to 0$ to evaluate this constant.

These important identities will be revisited in Section 4.4.

6. a) Verify Schlafli's form of the modular equation of degree 5,

(4.1.27) $$\left(\frac{u}{v}\right)^3 + \left(\frac{v}{u}\right)^3 = 2\left(u^2v^2 - \frac{1}{u^2v^2}\right)$$

where $u := 2^{-1/4}f(\tau)$ and $v := 2^{-1/4}f(5\tau)$, f as in (3.2.9).

b) Compute the corresponding equation for f_1.

4.2 *AN ELEMENTARY TRANSCENDENTAL APPROACH TO HIGHER ORDER TRANSFORMATIONS*

In terms of the nome q we have, by Theorem 2.3, the identification

(4.2.1) $$k(q) := k = \frac{\theta_2^2(q)}{\theta_3^2(q)}$$

(4.2.2) $$k'(q) := k' = \frac{\theta_4^2(q)}{\theta_3^2(q)}$$

(4.2.3) $$K(k) = \frac{\pi}{2}\,\theta_3^2(q)$$

and

(4.2.4) $$q = e^{-\pi K'(k)/K(k)}\,.$$

From Exercise 1e) of Section 1.4 and Exercise 5 of Section 4.1 we see that the quadratic modular equation (4.1.3) is satisfied by $l := k(q^{1/2})$ and $k := k(q)$, while the cubic equation is solved by $l := k(q^{1/3})$ and $k := k(q)$ and the quintic equation is solved by $l := k(q^{1/5})$ and $k := k(q)$. [To see this just observe that (4.2.4) uniquely determines q.] In general we will see in the next sections that the pth-order modular equation for k is a polynomial in two variables with integer coefficients that is satisfied by $k(q^p)$ and $k(q)$. We observe from (4.2.4) that for these algebraically connected moduli

(4.2.5)
$$p\,\frac{K'(k(q))}{K(k(q))} = \frac{K'(k(q^p))}{K(k(q^p))}\,.$$

Before turning to the general theory we wish to give an elementary derivation of the cubic transformation in theta function terms. From (4.1.16) the cubic modular equation for k is

(4.2.6)
$$\sqrt{kl} + \sqrt{k'l'} = 1\,.$$

From the preceding discussion this is seen to be equivalent to:

Theorem 4.1

(4.2.7)
$$\theta_4(q)\theta_4(q^3) + \theta_2(q)\theta_2(q^3) = \theta_3(q)\theta_3(q^3)\,.$$

Proof. From the definitions and Exercise 1 of Section 2.1 applied to $q^{n^2+3m^2}$ and $(-1)^{n+m}q^{n^2+3m^2}$ we have

$$\theta_3(q)\theta_3(q^3) = \sum_{h,j=-\infty}^{\infty} q^{(h+j)^2+3(h-j)^2} + \sum_{h,j=-\infty}^{\infty} q^{(h+j+1)^2+3(h-j)^2}$$

and

$$\theta_4(q)\theta_4(q^3) = \sum_{h,j=-\infty}^{\infty} q^{(h+j)^2+3(h-j)^2} - \sum_{h,j=-\infty}^{\infty} q^{(h+j+1)^2+3(h-j)^2}\,.$$

Now

$$(h+j+1)^2 + 3(h-j)^2 = (2h-j+\tfrac{1}{2})^2 + 3(j+\tfrac{1}{2})^2\,.$$

Thus subtraction of the two theta identities produces

$$\theta_3(q)\theta_3(q^3) - \theta_4(q)\theta_4(q^3) = 2\sum_{\substack{m,n=-\infty\\ m+n \text{ even}}}^{\infty} q^{(m+\frac{1}{2})^2+3(n+\frac{1}{2})^2}$$
$$= \theta_2(q)\theta_2(q^3)$$

(as replacing m by $1-m$ shows). □

Comments and Exercises

This is as far as we wish to pursue the transformation theory on an ad hoc basis. The next section introduces enough of the theory of modular functions to provide a general framework for the development of modular equations. We have only considered modular equations for p a prime. If we view the modular equation as the algebraic relation between $k(q^n)$ and $k(q)$ and can find this relation for p a prime, then for composite n a relationship

can be constructed out of the modular equations corresponding to the prime factors of n. Rational n are treated similarly.

1. Construct modular equations of order 4, 6, and 8 [that is, construct algebraic relationships that are satisfied by $k(q)$ and $k(q^2)$, $k(q^6)$, and $k(q^8)$, respectively].

2. Show, for

$$c := \frac{\pi}{2}\frac{K'}{K}(k(q))$$

that

$$0 \le k(q^{p^n}) \le 4e^{-cp^n} \qquad q \in (0,1)$$

and that

$$k(q^{p^n}) \sim 4e^{-cp^n} \qquad \text{as} \qquad n \to \infty\,.$$

Many modular identities follow from:

3. (*Schröter's formula*) Consider a general theta function written as

$$T(x,q) := \sum_{n=-\infty}^{\infty} x^n q^{n^2}$$

where $x \ne 0$, $|q|<1$ (as in Section 3.1). Let a and b be positive integers.

a) Show that

(4.2.8)
$$T(x,q^a)T(y,q^b) = \sum_{k=0}^{a+b-1} y^k q^{bk^2} T(xyq^{2bk}, q^{a+b})\,T(y^a x^{-b} q^{2abk}, q^{ab(a+b)})\,.$$

Hint: Write

$$T(x,q^a)T(y,q^b) = \sum_{m,n} x^m y^n q^{am^2+bn^2}$$

Let s be chosen so that $n = m + (a+b)s + k$ $(0 \le k < a+b)$ and let $u := m + bs$. Then u and s range over $\mathbb{Z}$ as m and n do. Also

$$x^m y^n = (xy)^u (x^{-b}y^a)^s y^k$$

and

$$am^2 + bn^2 = (a+b)u^2 + 2bku + ab(a+b)s^2 + 2abks + bk^2\,.$$

Now rearrange. (See Tannery and Molk [1893].)

b) A form of the seventh-order modular equation is

$$\sqrt{\theta_3(q)\theta_3(q^7)} - \sqrt{\theta_4(q)\theta_4(q^7)} = \sqrt{\theta_2(q)\theta_2(q^7)}\,.$$

(See (4.5.4).)
Use part a) with $a := 7$ and $b := 1$ to establish this formula.
Hint: Set $x := y := \pm 1$ to find a formula for $\theta_3(q)\theta_3(q^7) + \theta_4(q)\theta_4(q^7)$. Now set $x := y^7 := \pm q^7$ to similarly write $\theta_2(q)\theta_2(q^7) + \theta_2(-q)\theta_2(-q^7) = \theta_2(q)\theta_2(q^7)$. On making simple rearrangements this yields

$$\begin{aligned}\theta_3\theta_3(q^7) + \theta_4\theta_4(q^7) = 2T(1, q^8)T(1, q^{56})\\ + 2q^{16}T(q^8, q^8)T(q^{56}, q^{56})\\ + 4q^4T(q^4, q^8)T(q^{28}, q^{56})\end{aligned}$$

and

$$\begin{aligned}\theta_2\theta_2(q^7) = 2q^2T(q^8, q^8)T(1, q^{56}) + 2q^{14}T(1, q^8)T(q^{56}, q^{56})\\ + 4q^4T(q^4, q^8)T(q^{28}, q^{56})\,.\end{aligned}$$

Since $q^2T(q^8, q^8) = \theta_2(q^8)$ and $T(1, q^8) = \theta_3(q^8)$, we may write

$$\theta_3\theta_3(q^7) + \theta_4\theta_4(q^7) - \theta_2\theta_2(q^7) =$$

$$2[\theta_3(q^8) - \theta_2(q^8)][\theta_3(q^{56}) - \theta_2(q^{56})] = 2\theta_4(q^2)\theta_4(q^{14})\,.$$

Thus an application of equation (2.1.7ii) gives

$$(\sqrt{\theta_3\theta_3(q^7)} - \sqrt{\theta_4\theta_4(q^7)})^2 = \theta_2\theta_2(q^7)$$

as required.

c) Establish the cubic modular equation (4.2.7) as above.

4.3 *ELLIPTIC MODULAR FUNCTIONS*

The theory of elliptic modular functions and more general automorphic functions is, in part, a natural extension of the theory of elliptic functions. The basic defining property of elliptic functions is their invariance under a group of linear transformations. Automorphic functions are functions meromorphic in the upper half-plane $\mathscr{H} := \{\text{im(t)} > 0\}$ that are invariant under a group of linear fractional transformations. We will, of necessity, explore only the rudiments of this remarkable and difficult theory.

Definition 4.1

(*a*) The (inhomogeneous) *modular group* Γ (Γ-*group*) is the set of all transformations of the form

$$w = \frac{at+b}{ct+d} \qquad a, b, c, d \text{ integers}, \quad ad - bc = 1\,.$$

(*b*) The λ-group is the subgroup λ of Γ with a, d odd and b, c even.

That both of the above are groups (under composition) is straightforward. The transformation

$$w = \frac{at+b}{ct+d}$$

can be represented as either of the two matrices

$$\pm\begin{pmatrix} a & b \\ c & d\end{pmatrix}$$

and the group product becomes matrix multiplication (See Exercise 1.). The (homogeneous) modular group SL(2, $\mathbb{Z}$) distinguishes these matrices. Note that any element of the modular group fixes the real axis and maps $\mathscr{H}$ onto itself.

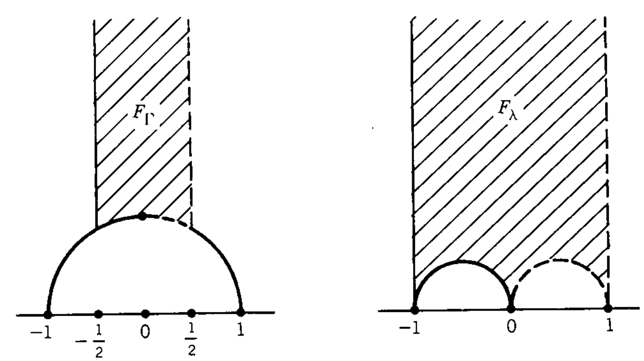
Definition 4.2

(*a*) The set F_Γ of $t \in \mathscr{H}^* := \{\text{im}(t) > 0\} \cup \{i\infty\} \cup \{\mathbb{Q}\}$ is defined by

$$F_\Gamma := \{|\text{re}(t)| < \tfrac{1}{2} \text{ and } |t| > 1\} \cup \{\text{re}(t) = -\tfrac{1}{2} \text{ and } |t| \geq 1\} \cup \{|t| = 1 \text{ and } -\tfrac{1}{2} \leq \text{re}(t) \leq 0\}\,.$$

(*b*) The set F_λ of $t \in \mathscr{H}^*$ is defined by

$$F_\lambda := \{|\text{re}(t)| < 1 \text{ and } |2t \pm 1| > 1\} \cup \{\text{re}(t) = -1\} \cup \{|2t+1| = 1\}\,.$$



These two sets described in a) and b) are *fundamental sets* for the Γ- and λ-groups. The interiors of these two sets (F^0_Γ and F^0_λ) are *fundamental regions* in the following sense.

Theorem 4.2

(a) Every point in $\mathcal{H}$ is the image under some element of Γ of some point of F_Γ.

If $A \in \Gamma$ is not the identity, then $A(F_\Gamma^0) \cap F_\Gamma^0 = \emptyset$.

(b) Every point in $\mathcal{H}$ is the image under some element of the λ-group of exactly one point of F_λ.

If $a \in \lambda$ is not the identity, then $A(F_\lambda^0) \cap F_\lambda^0 = \emptyset$.

The proof of this theorem is elementary though not entirely straightforward. (See Exercise 2.) Any set F (with interior F^0) which satisfies (a) or (b) of the above theorem is also a fundamental set.

Definition 4.3

(a) A Γ-*modular function* is a function f which satisfies:
 (i) f is meromorphic in $\mathcal{H}$.
 (ii) $f(A(t)) = f(t)$ for all $t \in \mathcal{H}^*$ and $A \in \Gamma$.
 (iii) $f(t)$ tends to a limit [possibly infinite in the sense that $1/f(t) \to 0$] as t tends to the vertices of the fundamental region F_Γ where the approach is from within the fundamental region F_Γ^0. [In the case of $i\infty$ the convergence is uniform in $\operatorname{re}(x+iy)$ as $y \to \infty$.] The vertices of the fundamental region are $(0, 1)$, $(-1/2, \sqrt{3}/2)$ and $i\infty$. Since f is meromorphic in $\mathcal{H}$, this condition is automatically satisfied at $(0, 1)$ and $(-1/2, \sqrt{3}/2)$ and need only be checked at $i\infty$.

(b) A λ-*modular function* is a function f which satisfies (i), (ii), and (iii) above with the Γ-group replaced by the λ-group. For condition (iii) the vertices of the fundamental region F_λ^0 are $(-1, 0)$, $(0, 0)$, and $i\infty$.

Our notation is not entirely standard. What we have termed Γ-modular is often just called modular or automorphic with respect to the Γ-group, while what we have labelled as λ-modular is often referred to as automorphic or modular with respect to the λ-group.

The existence of a λ-modular function is the content of the following theorem.

Theorem 4.3

The function

$$\lambda(t) := k^2(t) = \left[\frac{\theta_2(q)}{\theta_3(q)}\right]^4 \qquad q := e^{i\pi t}$$

is a λ-modular function.

Proof. From Corollary 3.1 we have

$$\lambda(t) = 16q \prod_{n=1}^{\infty} \left(\frac{1+q^{2n}}{1+q^{2n-1}}\right)^8 \tag{4.3.1}$$

and it is clear that λ is meromorphic in $\mathcal{H}$. For the invariance of λ under the λ-group it suffices, by Exercise 1e), to show that

$$\lambda(t+2) = \lambda(t) \tag{4.3.2}$$

and

$$\lambda\left(\frac{t}{2t+1}\right) = \lambda(t)\,. \tag{4.3.3}$$

The first equation follows since $e^{\pi it} = e^{\pi i(t+2)}$. The second equation is a consequence of (2.3.1), (2.3.3), and (2.1.10), which combine to yield

$$\lambda\left(-\frac{1}{t}\right) = 1 - \lambda(t)\,. \tag{4.3.4}$$

(Note that $t = is$.) Hence

$$\lambda\left(\frac{t}{2t+1}\right) = \lambda\left(\frac{1}{2+1/t}\right) = 1 - \lambda\left(-2-\frac{1}{t}\right) = 1 - \lambda\left(-\frac{1}{t}\right) = \lambda(t)\,.$$

Finally we observe that, in a limiting sense,

$$\lambda(i\infty) = 0 \qquad \lambda(0) = 1 \qquad \lambda(\pm 1) = \infty\,. \tag{4.3.5}$$

The first value is immediate from (4.3.1), while the value at zero can be calculated from (4.3.4). (Observe that as $t \to 0$ in F_λ, $1/t \to \infty$ in F_λ.) The value at 1 is computed from Jacobi's imaginary transformation

$$\lambda(t+1) = \frac{\lambda(t)}{\lambda(t)-1}\,. \tag{4.3.6}$$

(See Exercise 4.) □

Some additional properties of λ are established in Exercises 4, 5, and 10. From (4.3.4) and (4.3.6) one can prove, as in Exercise 6, the following theorem.

Theorem 4.4

The function

$$J(t) := \frac{4}{27}\,\frac{[1-\lambda(t)+\lambda^2(t)]^3}{\lambda^2(t)[1-\lambda(t)]^2} = \frac{4}{27}\,\frac{\{1-[k(t)k'(t)]^2\}^3}{[k(t)k'(t)]^4}$$

is Γ-modular. J is called Klein's *absolute invariant*.

The basic result we need is a version of Liouville's theorem.

Theorem 4.5

A Γ-modular function that is bounded on F_Γ is constant. Similarly, a λ-modular function that is bounded on F_λ is constant.

Proof. Suppose f is Γ-modular and is bounded and nonconstant on F_Γ. By Theorem 4.2 this implies that f is analytic on $\mathscr{H}$. Consider $f(t)-f(i\infty)$. This function has no poles interior to F_Γ, and so achieves its maximum modulus at some finite point on the boundary of F_Γ. By the invariance of $f-f(i\infty)$ under Γ this is a global maximum at an interior point of $\mathscr{H}$, which is impossible.

For the second part consider the λ-modular function

$$[f(t)-f(0)][f(t)-f(-1)][f(t)-f(i\infty)]. \quad \square$$

This is sufficient theory for our discussion of modular equations in the next section.

Comments and Exercises

This is only the very tip of the iceberg. We have restricted our attention to two particular groups where we can directly establish the existence of modular functions. In general this restriction is unnecessary. Only slightly further into the theory are results such as: any modular function takes each complex value the same number of times in the fundamental region. An important consequence of this is that λ takes every value exactly once in F_λ and λ has a well-defined inverse that has branch points only at 0, 1, and ∞ (Exercise 10). J has similar properties on F_Γ. One can now prove, much as for elliptic functions, that two nonconstant functions which are modular with respect to the same group are algebraically connected. Furthermore, if one of these functions is univalent on the fundamental region, then the other is a rational function of it.

This wide-ranging and difficult body of theory that is intimately tied in to many questions in number theory and algebraic geometry may be pursued in any number of texts, such as Apostol [76*b*], Chandrasekharan [85], Lang [73], Lehner [66], Rankin [77], or Schoeneberg [76].

Two of the seminal papers of the subject, both dating from 1882, are due to Klein and Poincaré (selections of which may be found in Birkhoff [73]). Poincaré was interested in studying linear differential equations with algebraic coefficients. Klein, who considered this his main field of work, in keeping with his Erlanger Programme had more algebraic and geometric interests (Klein and Fricke [1892]).

1. a) Verify that Γ and λ are groups.

b) Verify that composition of transformations is equivalent to multiplication of the associated matrices.

c) Show that two transformations represent the same function if and only if they have the same coefficients (associated matrix up to sign).

d) Show that Γ is generated by

$$S_\Gamma := \begin{pmatrix} 1 & 1 \\ 0 & 1 \end{pmatrix} \quad \text{and} \quad T_\Gamma := \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}.$$

e) Show that λ is generated by

$$S_\lambda := \begin{pmatrix} 1 & 2 \\ 0 & 1 \end{pmatrix} \quad \text{and} \quad T_\lambda := \begin{pmatrix} 1 & 0 \\ 2 & 1 \end{pmatrix}.$$

2. Prove Theorem 4.2.

a) *Hint*: To prove part (*a*), fix $z \in \mathscr{H}$ and let $A = \begin{pmatrix} a & b \\ c & d \end{pmatrix} \in \Gamma$. Show that

$$\operatorname{im} A(z) = \frac{\operatorname{im}(z)}{|cz+d|^2}.$$

Pick any element of Γ that minimizes $|cz+d|$ and let w be the image of z under this transformation. By considering $T_\Gamma(w)$ show that $|w| \geq 1$ and by considering $S_\Gamma^{(k)}(w)$ show that for some k, $|\operatorname{re}[S^{(k)}(w)]| \leq \frac{1}{2}$. For this k, $|S^{(k)}(w)| \geq 1$. Thus every element of $\mathscr{H}$ is the image of some element of F_Γ.

b) Show that no two elements of F_Γ^0 map to each other under an element of Γ. Examine the image of F_Γ under S_Γ and T_Γ.

c) Deduce part (*b*) of Theorem 4.2 from part (*a*).

3. The upper half-plane can be tesselated by images of the fundamental region under the generating transformations. Sketch pictures of the tesselations associated with the Γ-group and the λ-group.

4. a) Show that $\lambda(A)$ is transformed into one of $\lambda, 1-\lambda, 1/\lambda, 1/(1-\lambda)$, $\lambda/(\lambda-1)$, $1-1/\lambda$ by any $A \in \Gamma$. *Hint*: Examine $\lambda(t+1)$ and $\lambda(-1/t)$ using similar arguments to those of Theorem 4.3. Use Exercise 1d).

b) Show that $\lambda(m/n)=0$, $\gcd(m,n)=1$, if and only if m is odd and n is even.

5. Show that with $q := e^{i\pi t}$,

$$\frac{16}{\lambda(t)} = \frac{1}{q} + \sum_{n=0}^{\infty} b_n q^n$$

where the b_n are integers. Show that $1/\lambda(t)$ is finite at every point of $F_\Gamma - \{i\infty\}$.

6. a) Prove Theorem 4.4 from (4.3.4) and (4.3.6).

b) Let $\bar{q} := e^{2\pi i t}$. Show that

$$j(t) := 1728J(t) = \frac{1}{\bar{q}} + \sum_{n=0}^{\infty} c_n \bar{q}^n$$

where the c_n are integers. [In fact, $\bar{q}j(t) = Q_1^{48}(256\bar{q} + Q_1^{-24})^3$.]

c) Show that $f^{24}(t)$, $-f_1^{24}(t)$, and $-f_2^{24}(t)$ are the roots of

$$(x-16)^3 - xj(t) = 0 .$$

[See (3.2.9) for definitions.]

7. a) Show that if f is Γ-modular then for some integer k and nonzero constant c

$$f(t) \sim ce^{2ki\pi t}$$

as $t \to i\infty$.

Hint: Let $\hat{f}(\bar{q}) := f(t)$ where $\bar{q} := e^{2\pi i t}$ for t in F_Γ. Show, by modularity of f, that $\hat{f}$ is meromorphic in $\bar{q}$ in a neighbourhood of zero. Show also that $\hat{f}$ has a pole at zero. Thus f has a convergent $\bar{q}$-expansion at $i\infty$ with finite principal part.

b) Show that the Γ-modular functions form a field. Likewise the λ-modular functions.

8. Establish that f_1^{24}, f_2^{24}, and f^{24} [see (3.2.9) for definitions] are λ-modular.

9. The Schwartz derivative of any function f is

$$S(f) := \frac{2\dot{f}\dddot{f} - 3(\ddot{f})^2}{2(\dot{f})^2} .$$

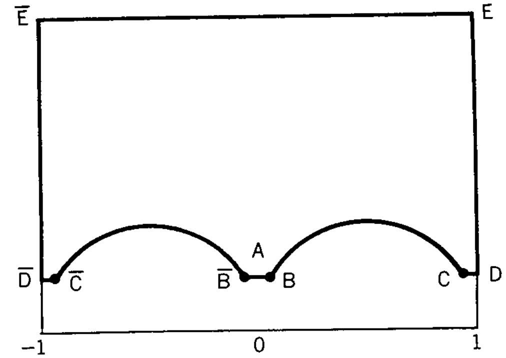
Show that if f is modular, then so is $S(f)/(\dot{f})^2$. Show that $\dot{f}$ is not in general modular.

10. (*On the inverse of* λ)

a) Show that λ maps the set $A := \{\mathrm{re}(z) = -1, 0 < \mathrm{im}\, z\}$ one to one onto $(-\infty, 0)$. *Hint*: $\lambda(t \pm 1) = \lambda(t)/[\lambda(t) - 1]$. Now consider λ on the imaginary axis.

b) Show that λ maps the semicircle $B := \{|z + \frac{1}{2}| = \frac{1}{2}, \mathrm{im}(z) > 0\}$ one to one onto $(1, \infty)$. *Hint*: $\lambda(-1/t) = 1 - \lambda(t)$.

c) Show that λ maps the interior of F_λ one to one onto $\mathbb{C} -$



$\{(-\infty, 0] \cup [1, \infty)\}$. *Hint*: The number of zeros of $\lambda - c$ is

$$\frac{1}{2\pi i}\int_\gamma \frac{\lambda'(t)}{\lambda(t) - c}\, dz$$

where γ is a contour of the form seen in the accompanying figure. Use the invariance $\lambda(t) = \lambda(t+2)$ to estimate the integral on the sides of the contour. Use the relation $\lambda(-1/t) = 1 - \lambda(t)$ to relate the integral on BC to the integral on $\bar{E}\bar{D}$. Use the relation $\lambda(t \pm 1) = \lambda(t)/[\lambda(t) - 1]$ to estimate the integral on CD and $\bar{D}\bar{C}$ in terms of $\bar{B}AB$ and then (by $t \to -1/t$) in terms of $\bar{E}E$. Finally take limits.

d) Thus with respect to F_Γ, λ has a well-defined analytic inverse with branch points at $0, 1$ and ∞.

11. (*Picard's theorem*) Show that a nonconstant entire function assumes every complex value except possibly one.

Hint: Suppose F does not assume either α or β, then $G(z) := [F(z) - \alpha]/(\beta - \alpha)$ never assumes 0 or 1. If $\omega := \lambda^{-1}$, then $\omega(G(z))$ is entire (by analytic continuation). Show that $\omega(G(z))$ is constant since $\omega(G(z)) \in \{\mathrm{im}(z) \geq 0\}$ and hence $e^{\omega(G(z))}$ is a bounded entire function.

It is worth observing that the apparently special case analysis of the function λ leads directly to the celebrated general theorem of Picard.

4.4 *THE MODULAR EQUATIONS FOR λ AND j*

A *transformation of order p* is a matrix

(4.4.1) $$\begin{pmatrix} a & b \\ c & d \end{pmatrix} \qquad a, b, c, d \text{ integers}, \quad ad - bc = p$$

or the associated linear fractional transformation. We assume throughout that p is an odd prime, though for much of the development this is unnecessary. We will denote the set of all such transformations by T_p. We say that M is equivalent to N mod G ($M \equiv N \bmod G$) for a group of transformations G if there is an $S \in G$ so that $M = SN$. We need the following purely algebraic result.

Lemma 4.1

(*a*) Every $M \in T_p$ is equivalent mod Γ to one of the $p+1$ transformations of the set $\mathscr{A}$, where

$$\mathscr{A} := \left\{ A_p := \begin{pmatrix} p & 0 \\ 0 & 1 \end{pmatrix},\ A_i := \begin{pmatrix} 1 & i \\ 0 & p \end{pmatrix}, i = 0, 1, \ldots, p-1 \right\}.$$

(*b*) The $p+1$ elements of $\mathscr{A}$ are pairwise inequivalent mod Γ.

(*c*) Every B of the form $B := B_i C$, where C is in the λ-group and $B_i \in \mathscr{B}$, is equivalent mod λ to some element of $\mathscr{B}$, where

$$\mathscr{B} := \left\{ B_p := \begin{pmatrix} p & 0 \\ 0 & 1 \end{pmatrix},\ B_i := \begin{pmatrix} 1 & 2i \\ 0 & p \end{pmatrix},\ i = 0, 1, \ldots, p-1 \right\},$$

(*d*) The $p+1$ elements of $\mathscr{B}$ are pairwise inequivalent mod λ.

The proof is left as Exercise 1.

Theorem 4.6

(*a*) The $p+1$ functions

$$J(A_i(t)) \qquad i = 0, \ldots, p$$

are permuted by any element of the Γ-group.

(*b*) The $p+1$ functions

$$\lambda(B_i(t)) \qquad i = 0, \ldots, p$$

are permuted by any element of the λ-group.

Proof. For part (*a*) we must show that $\{J \circ A_i \circ S\}_{i=1}^{p} = \{J \circ A_i\}_{i=1}^{p}$ for any $S \in \Gamma$. We first observe by the lemma that if $S \in \Gamma$, then since $A_i S \in T_p$,

$$A_i S \equiv A_j \bmod \Gamma \qquad \text{for some } j$$

Thus by the modularity of J,

$$J \circ A_i \circ S = J \circ A_j$$

which with part (*b*) of the lemma finishes the proof. The second part is identical via parts (*c*) and (*d*) of the lemma. □

The *modular equation for* λ of order p is the polynomial

$$(4.4.2) \qquad W_p(x, \lambda) := \prod_{i=0}^{p} (x - \lambda_i) \qquad \lambda_i := \lambda \circ B_i\,.$$

This is obviously of degree $p+1$ in x and has a root at each λ_i. Note that $\lambda_p(t) := \lambda(pt)$ and $\lambda_i(t) = \lambda((t+2i)/p)$, $i<p$. Thus as functions of q, $\lambda_p(q) = \lambda(q^p)$ and $\lambda_i(q) = \lambda(\alpha^i q^{1/p})$, where $\alpha^p = 1$. We now show that (*independent* of t) W_p is also a polynomial in λ. This relies on two basic facts. First, any symmetric polynomial in the λ_i is λ-modular and second, any λ-modular function is a rational function of λ.

Theorem 4.7

$W_p(x, \lambda)$ is a polynomial of degree $p+1$ in x and λ with integer coefficients. The coefficients of x^{p+1} and λ^{p+1} are both 1.

Proof. Consider $\bar{W}_p(x, \lambda) := \Pi_{i=0}^{p} (y - \bar{\lambda}_i)$, where $\bar{\lambda}_i := 16/\lambda_i$ and $y := 16/x$. This is a convenient form to work with. Observe that W_p and $\bar{W}_p$ are connected by

$$(4.4.3) \qquad 16^{p+1} W_p(x, \lambda) = \left[x^{p+1} \prod_{i=0}^{p} \lambda_i \right] \bar{W}_p(x, \lambda)\,.$$

Now by Theorem 4.6 any symmetric polynomial in $\lambda_0^{-1}, \lambda_1^{-1}, \ldots, \lambda_p^{-1}$ is left invariant by any element of the λ-group. (See Exercise 6 of Section 11.2.) It follows that any such polynomial is λ-modular, and by Exercise 4b) of the last section $\bar{\lambda}_i$ is finite valued in the fundamental set except possibly at $t := i\infty$. In particular if s_i is the coefficient of y^i in W_p (viewed as a polynomial in y), then s_i is λ-modular. From Corollary 3.1,

$$(4.4.4) \qquad \lambda(q) = 16q \prod_{n=1}^{\infty} \left(\frac{1+q^{2n}}{1+q^{2n-1}} \right)^8$$

and we have integers a_n such that

$$\bar{\lambda} := \frac{16}{\lambda} = \frac{1}{q} + \sum_{n=0}^{\infty} a_n q^n$$

$$\bar{\lambda}_i = \frac{1}{\alpha^i q^{1/p}} + \sum_{n=0}^{\infty} a_n \alpha^{ni} q^{n/p} \qquad i<p$$

and

$$\bar{\lambda}_p = \frac{1}{q^p} + \sum_{n=0}^{\infty} a_n q^{np}$$

where α is a primitive pth root of unity. It can now be established that there are integers c_i so that

(4.4.5)
$$s_i = \sum_{i=-(p+1)}^{\infty} c_i q^i .$$

It is a consequence of the symmetry that the nonintegral powers of q vanish. (See Exercise 2.) Next there is a polynomial P of degree at most $p+1$ with integer coefficients so that

$$s_i - P(\bar{\lambda}) = \sum_{i=0}^{\infty} d_i q^i$$

and $s_i - P(\bar{\lambda})$ has zero principal part. This is easily proved. First remove the $q^{-(p+1)}$ term by considering

$$s_i - c_{-(p+1)}\bar{\lambda}^{p+1}$$

and then proceed inductively. Observe from (4.4.4) and (4.3.5) that the only candidate for a pole of $s_i - P(\bar{\lambda})$ is $q=0$ but P has been chosen so that $s_i - P(\bar{\lambda})$ is finite at $q=0$. Thus we see that $s_i - P(\bar{\lambda})$ is a *bounded* λ-modular function and is hence, by Theorem 4.5, constant. Since

$$\bar{\lambda} = \frac{16}{\lambda}$$

we have that s_i is a polynomial of degree at most $p+1$ in $\bar{\lambda} := 16/\lambda$ with integer coefficients. Hence $\bar{W}_p(x, \lambda)$ is a polynomial of degree $p+1$ in $16/x$ and $16/\lambda$ with integer coefficients. We can prove directly (see Exercise 3) that

$$\prod_{i=0}^{p} \lambda_i = \lambda^{p+1} .$$

Exercise 7 shows that 16^{p+1} divides every coefficient of $\bar{W}_p(x, \lambda)$ when viewed as a polynomial in $1/x$ and $1/\lambda$. Thus with (4.4.3),

$$W_p(x, \lambda) = \frac{x^{p+1}\lambda^{p+1}}{16^{p+1}} \bar{W}_p(x, \lambda)$$

is of the required form. □

Analogously we have a modular equation for $j := 1728\,J$. (See Exercise 4.)

***Theorem* 4.8**

The *modular equation for j* of order p

(4.4.6)
$$F_p(x, j) := \prod_{i=0}^{p} (x - j_i) \qquad j_i := j \circ A_i$$

is a polynomial with integer coefficients of degree $p+1$ in x and j. The coefficients of x^{p+1} and j^{p+1} are both 1.

The modular equation (4.4.2) is irreducible over $\mathbb{C}(\lambda)$ (the rational functions in λ) since any root can be transformed into any other by an appropriate transformation. (See Exercise 5.) Likewise (4.4.6) is irreducible over the rational functions in j. The Galois group of F_p over $\mathbb{Q}_p(j)$ is a group of order $p(p^2-1)/2$, which is nonsolvable for $p \ge 5$. (See Exercise 6.) Here $\mathbb{Q}_p$ is $\mathbb{Q}$ adjoin the pth roots of unity. For nonprime n, modular equations can be constructed from the modular equations corresponding to the prime factors of n. (See Exercise 8.)

Comments and Exercises

Further properties of modular equations are chronicled in Lang [73], Schoeneberg [76], and particularly in Weber [08]. We have chosen a path of limited generality focusing on the modular equations for λ and j. It should however be fairly clear that analogous equations hold for other modular functions.

1. Prove Lemma 4.1.
Hint: For (*a*) prove that M is equivalent to an upper triangular matrix mod Γ. Then write out the system of equations required for two triangular matrices to be equivalent. For part (*c*) show that B_iC is equivalent to a triangular matrix mod λ. Note that B_iC has determinant p, and hence the diagonal entries of this equivalent triangular matrix are ± 1, $\pm$p.

2. a) Suppose that

$$f(q) := \sum_{n=-h}^{\infty} c_n q^n \qquad c_n \text{ real} .$$

Show, for $\alpha := e^{2\pi i/p}$ and p prime, that

$$\sum_{n=1}^{p} [f(\alpha^n q^{n/p})]^m \qquad m \text{ integer}$$

has no fractional powers of q in its expansion. (See Exercise 4 of Section 6.2.)

b) Prove that (4.4.5) holds by applying Newton's formulae to express s_i in terms of powers of the roots. (See Exercise 6 of Section 11.2.)

3. Show directly from (4.4.4) that

$$\prod_{i=0}^{p} \lambda_i = \lambda^{p+1}.$$

4. Prove Theorem 4.8 by modifying the proof of Theorem 4.7. Use Exercise 6b) of section 4.3. The proof is somewhat easier since we can consider $\Pi_{i=0}^{p}(x - j_i)$ directly.
5. Show that the modular equations (4.4.2) and (4.4.6) are irreducible in x, over $\mathbb{C}(\lambda)$ and $\mathbb{C}(j)$, respectively, by elaborating on the comments following Theorem 4.8. This requires a minimal knowledge of Galois theory. Note that the transformations of Lemma 4.1 act transitively on the roots.

6. Show that
a) $W_p(x, 1) = (x-1)^{p+1}$
b) $W_p(x, 0) = x^{p+1}$.

Hint: Consider the orbits of 0 and $i\infty$ under the λ-group.

7. a) Show that

$$W_p(x, \lambda) = W_p(\lambda, x)$$

and

$$W_p(x, \lambda) = W_p\left(\frac{1}{\lambda}, \frac{1}{x}\right) x^{p+1} \lambda^{p+1}$$

and if $c_{i,j}$ is the coefficient of $x^i \lambda^j$ in W_p, then

$$c_{i,j} = c_{p+1-i,p+1-j} = c_{j,i} = c_{p+1-j,p+1-i}.$$

Thus there is a fourfold symmetry in the coefficients of W_p.
Hint: $W_p(\lambda(q^p), \lambda(q)) = 0$ and $W_p(\lambda(q), \lambda(q^p)) = 0$ and by Exercise 5, $W_p(x, \lambda)$ is irreducible in x over $\mathbb{C}(\lambda)$. Also, $W_p(x, \lambda)$ and $W_p(\lambda, x)$ have a common root $x = \lambda(q^p)$ and are of the same degree in x. Hence,

$$W_p(x, \lambda) = R(\lambda) W_p(\lambda, x)$$

where R is a rational function of λ. Show that this implies that $R \equiv 1$. For the second symmetry use $\lambda(t/(t-1)) = 1/\lambda(t)$.
b) Consider $W_p(x, \lambda)$, as in the proof of Theorem 4.7, as a polynomial in $1/x$ and $1/\lambda$. Let $\bar{c}_{i,j}$ be the coefficient of $x^{-i}\lambda^{-j}$. Show directly that

$$16^{i+j} | \bar{c}_{i,j} \qquad i + j \geq p + 1$$

and, by part a), that

$$16^{2(p+1)-(i+j)} | \bar{c}_{i,j} \qquad i + j \leq p.$$

c) Show that the coefficient of $x^i \lambda^j$ in $W_p(x, \lambda)$ is divisible by $16^{|p+1-(i+j)|}$.

8. In general, for n not necessarily prime, the modular equation (4.4.2) has degree $\psi(n) := n \prod_{p|n}(1 + 1/p)$. Let $n := p_1 \cdots p_k$ be a product of distinct primes. Prove that there exists a two-variable polynomial $W_n(x, y)$ of degree at most $\psi(n)$ that satisfies

$$W_n(\lambda(q), \lambda(q^n)) = 0.$$

Hint: Let $n = p_1 p_2$. Since

$$W_{p_1}(\lambda(q^{p_1}), \lambda(q)) = 0$$

and

$$W_{p_2}(\lambda(q^{p_1 p_2}), \lambda(q^{p_1})) = 0$$

we deduce that $\lambda(q^{p_1 p_2})$ is algebraic over $\mathbb{Q}(\lambda(q))$ and is of degree $\psi(p_1 p_2)$. Now proceed inductively.

9. Show that the coefficients of $W_3(x, \lambda)$ are

	x^4	x^3	x^2	x^1	1
λ^4					1
λ^3		−256	384	−132	
λ^2		384	−762	384	
λ^1		−132	384	−256	
1	1				

Note that by Exercises 6 and 7 is suffices to determine $c_{1,1}$ and $c_{1,2}$. The $c_{1,1}$ coefficient is always -16^{p-1}. (See Exercise 6 of the next section.)

10. (*On the Galois group* of F_p) If $A \in \Gamma$ then A induces an automorphism on the j_i that fixes j. Hence A is an element of the splitting field for F_p over $\mathbb{Q}(j)$. Any two elements S and T of Γ induce the same automorphism exactly when

$$ST^{-1} \equiv \begin{pmatrix} \alpha & 0 \\ 0 & \alpha \end{pmatrix} \pmod{p}$$

for some α. Equivalently $MST^{-1}M \in \Gamma$ for all $M \in T_p$. One can show that Γ, equivalenced as above, is the Galois group for F_p over $\mathbb{Q}_p(j)$ and that it is a group of order $p(p^2-1)/2$ which is nonsolvable for $p \geq 5$. (See Klein and Fricke [1892], Schoeneberg [76], and Exercise 8 of Section 4.5.)

4.5 *THE MODULAR EQUATION IN* $u-v$ *FORM*

The actual calculation of the modular relation for λ is most readily carried out in the associated variables $u := k^{1/4} := \lambda^{1/8}$ and $v := l^{1/4} := x^{1/8}$. Analogously to Theorem 4.7, though with a few substantial additional details (see Exercises 1 and 2), we have the following theorem.

Theorem 4.9

If p is an odd prime, then *the modular equation in u–v form* is given by

$$\Omega_p(v, u) := (v-u_0)(v-u_1)\cdots(v-u_p) \tag{4.5.1}$$

where

$$u_p := (-1)^{(p^2-1)/8}[\lambda(q^p)]^{1/8} := (-1)^{(p^2-1)/8}u(q^p) \qquad q := e^{i\pi t}$$
$$u_k := [\lambda(\alpha^{8k}q^{1/p})]^{1/8} := u(\alpha^{8k}q^{1/p}) \qquad k = 0, 2, \ldots, p-1$$

and α is a primitive pth root of unity. This modular equation is a polynomial in u and v of degree $p+1$ (independent of t) with integer coefficients.

For $p \equiv \pm 1 \pmod 8$,

$$\Omega_p(v, 1) = (v-1)^{p+1}$$
$$\Omega_p(v, u) = \Omega_p(u, v) = \Omega_p(-v, -u)\,.$$

The coefficients of v^{p+1} and u^{p+1} are 1.

For $p \equiv \pm 3 \pmod 8$,

$$\Omega_p(v, 1) = (v+1)^p(v-1)$$
$$\Omega_p(v, u) = -\Omega_p(-u, v) = \Omega_p(-v, -u)\,.$$

The coefficient of u^{p+1} is -1 and the coefficient of v^{p+1} is 1.

The most striking property of the modular equation in u and v is the "octicity." Because $u_i(q^p)$ is of the form $\alpha^i q^{1/8} f(\alpha^{8i}q)$, where f is analytic in q, only every eighth coefficient of the modular equation is nonzero. (See Exercise 3.) We illustrate with some examples which give the nonzero coefficients and the column sums.

Ω_3

	v^4	v^3	v^2	v	1
u^4					−1
u^3		+2			
u^2					
u				−2	
1	+1				
	1	+2	0	−2	−1 $= (v+1)^3(v-1)$

Ω_5

	v^6	v^5	v^4	v^3	v^2	v	1
u^6							−1
u^5		+4					
u^4					−5		
u^3							
u^2			+5				
u						−4	
1	+1						
	1	+4	+5	0	−5	−4	−1 $= (v+1)^5(v-1)$

Ω_7

	v^8	v^7	v^6	v^5	v^4	v^3	v^2	v	1
u^8	0								+1
u^7		−8							
u^6			+28						
u^5				−56					
u^4					+70				
u^3						−56			
u^2							+28		
u								−8	
1	+1								0
	1	−8	+28	−56	+70	−56	+28	−8	+1 $= (v-1)^8$

Ω_{11}

	v^{12}	v^{11}	v^{10}	v^9	v^8	v^7	v^6	v^5	v^4	v^3	v^2	v	1
u^{12}					0								−1
u^{11}		+32								−22			
u^{10}							−44						
u^9				+88								+22	
u^8	0								−165				
u^7						+132							
u^6			+44								−44		
u^5								−132					
u^4					+165								0
u^3		−22								−88			
u^2							+44						
u				+22								−32	
1	+1								0				
	1	+10	+44	+110	+165	+132	0	−132	−165	−110	−44	−10	−1

$= (v+1)^{11}(v-1)$

Ω_{13}

	v^{14}	v^{13}	v^{12}	v^{11}	v^{10}	v^9	v^8	v^7	v^6	v^5	v^4	v^3	v^2	v	1
u^{14}							0								−1
u^{13}		+64								−52					
u^{12}					0								−65		
u^{11}								+208							
u^{10}			0								--429				
u^9						+520								+52	
u^8	0								−429						
u^7				+208								−208			
u^6							+429								0
u^5		−52								−520					
u^4					+429								0		
u^3								−208							
u^2			+65								0				
u						+52								−64	
1	1								0						
	1	+12	+65	+208	+429	+572	+429	0	−429	−572	−429	−208	−65	−12	−1

$= (v+1)^{13}(v-1)$

Ω_{17}

	v^{18}	v^{17}	v^{16}	v^{15}	v^{14}	v^{13}	v^{12}	v^{11}	v^{10}	v^{9}	v^{8}	v^{7}	v^{6}	v^{5}	v^{4}	v^{3}	v^{2}	v	1	
u^{18}			0								0								+1	
u^{17}		−256								+272								−34		
u^{16}	0								−272								425			
u^{15}								+1632								−2448				
u^{14}							−4080								+7140					
u^{13}						+4896								−13464						
u^{12}					−4080								+22644							
u^{11}				+1632								−33456								
u^{10}			−272								+44030								0	
u^{9}		+272								−49164								+272		
u^{8}	0								+44030								−272			
u^{7}								−33456								+1632				
u^{6}							+22644								−4080					
u^{5}						−13464								+4896						
u^{4}					+7140								−4080							
u^{3}				−2418								+1632								
u^{2}			+425								−272								0	
u		−34								+272								−256		
1	+1								0								0			
	1	−18	+153	−816	+3060	−8568	+18564	−31824	+43758	−48520	+43758	−31824	+18564	−8568	+3060	−816	+153	−18	+1	$= (v-1)^{18}$

	v^{20}	v^{19}	v^{18}	v^{17}	v^{16}	v^{15}	v^{14}	v^{13}	v^{12}	v^{11}	v^{10}	v^{9}	v^{8}	v^{7}	v^{6}	v^{5}	v^{4}	v^{3}	v^{2}	v	1	
u^{20}					0								0								−1	
u^{19}		+512								−608								+114				
u^{18}							+2432								−2584							
u^{17}				−2432								+3344								−114		
u^{16}	0								+3952								−6859					
u^{15}						+5472								+2280								
u^{14}			−2432								−10488								−2584			
u^{13}								+25536								−2280						
u^{12}					−3952								−21242								0	
u^{11}		−608								+20748								−3344				
u^{10}							+10488								−10488							
u^{9}				+3344								−20748								+608		
u^{8}									+21242								+3952					
u^{7}						+2280								−25536								
u^{6}			+2584								+10488								+2432			
u^{5}								−2280								−5472						
u^{4}					+6859								−3952								0	
u^{3}		+114								−3344								+2432				
u^{2}							+2584								−2432							
u				−114								+608							−512			
1	1								0								0					
	1	+18	+152	+798	+2907	+7752	+15504	+23256	+25194	+16796	0	−16796	−25194	−23256	−15504	−7752	−2907	−798	−152	−18	−1	$= (V+1)^{19}(V-1$

	v^{24}	v^{23}	v^{22}	v^{21}	v^{20}	v^{19}	v^{18}	v^{17}	v^{16}
u^{24}	0								
u^{23}		−2048							
u^{22}			0						
u^{21}				−23552					
u^{20}					+52992				
u^{19}						−138368			
u^{18}							+334144		
u^{17}								−712448	
u^{16}	0								1159200
u^{15}		+2944							
u^{14}			−13248						
u^{13}				+75072					
Ω_{23} u^{12}					−124752				
u^{11}						+149408			
u^{10}							−213072		
u^{9}								+367264	
u^{8}	0								−423729
u^{7}		−920							
u^{6}			+13524						
u^{5}				−53544					
u^{4}					+82386				
u^{3}						−53544			
u^{2}							+13524		
u								−920	
0	+1								0
	1	−24	+276	−2024	+10626	−42504	+134596	−346104	+735471

The exhibited portion of Ω_{23} is sufficient to easily calculate the remainder of the coefficients because of the symmetries. For $p \equiv \pm 1 \bmod 8$ the table is symmetric through both diagonals. For $p \equiv \pm 3 \bmod 8$ the reflections through the diagonals change the sign of the entries according to $c_{i,j} = (-1)^{i+1} c_{j,i}$ and $c_{i,j} = (-1)^i c_{p+1-j,p+1-i}$, where $c_{i,j}$ is the coefficient of $v^i u^j$ in Ω. (See Exercise 4.)

The numerical calculation of these modular equations is fairly straightforward. From the q expansions for the θ functions we can compute $u_0, u_1, \ldots, u_p$ for a variety of q values (for $p := 23$ one must use three values of q). We then use (4.5.1) to calculate the coefficient of v^i at these values. However, we know the form of the coefficient (for $p := 23$ and $i := 23$ one has, for example, that the coefficient of v^i is of the form $au^{23} + bu^{15} + cu^7$), and we can easily calculate u at the same q values we

used to calculate the coefficient of v^i. This leads to a system of linear equations to solve. We know that the system has an integral solution. We also know what the column sums are in each case. One can use this information to reduce the size of the system by 1 or, perhaps more reasonably, as a check on the solution.

The main limitation is that the size of the entries grows exponentially with p. The pth modular equation will have entries of size roughly 2^p, so for large examples one must work to a high degree of precision. Note that the size of the linear system only grows as $p/8$.

Comments and Exercises

A fairly complete account of modular equations up to 1928 is given in Hannah [28]. This includes equations of degree 103, 107, 127, 167, 191, and 239.

The $u - v$ modular equations up to degree 20 are presented in Cayley [1874] as we have presented them. We easily computed Ω_{23} by the method outlined in the section. The others were originally calculated by Sohnke (1836), whose method roughly parallels the one we have described, except, that he computed an expansion for $u(q)/q^{1/8}$ and computed sufficient coefficients of u^m, to calculate the elementary symmetric functions directly. Then instead of solving a linear system, he compares coefficients. As Cayley [1874] points out, "The process is a laborious one (although less so than perhaps might beforehand have been imagined)."

A particularly simple form of the modular equation for $p = 23$, due to Schröter, is

$$(kl)^{1/4} + (k'l')^{1/4} + 2^{2/3}(klk'l')^{1/12} = 1\,. \qquad (4.5.2)$$

For many theoretical purposes modular equations for j are preferable. However, for calculations the modular equation for u is usually simpler. The extent of the numerical simplification is quite remarkable. Du Val [73] exhibits low-order modular equations for the Γ-modular function $I := J/(J-1)$. The cubic modular equation for I tabulates as a 5×5 matrix where all but one of the 25 entries are either 15- or 16-digit integers. Modular equations for j up to order 11 have been calculated. (See Kaltofen and Yui [84].) For the 11th-order modular equation the coefficients are enormous. For example, the coefficient of j^6 is

$$270909647855313899315632002810352263119290522273O3$$

$$\times 2^{92} 3^{19} 5^{20} 11^2 \cdot 53\,.$$

Various of the λ and j modular equations are presented in Greenhill [1892]. In particular, clean forms for $p = 29$, 31, 47, and 71 are given for W_p.

Exercises 1 and 2 outline the proof of Theorem 4.9. Some of the details are rather complicated. The flavour should come through.

1. a) Observe using (3.2.3) that

$$u(q)=\sqrt{2}q^{1/8}\prod_{n=1}^{\infty}\left(\frac{1+q^{2n}}{1+q^{2n-1}}\right)\qquad q:=e^{i\pi t}.$$

b) Analyze the action of λ-group on u. Show that

$$u\circ S_\lambda^{(8)}=u \qquad\text{and}\qquad u\circ T_\lambda=u\,.$$

Observe that $u\circ S_\lambda=\beta u$ where β is an eight root of unity.

c) Analyze the action that S_λ induces on the functions $\lambda_0,\ldots,\lambda_p$ and on the functions $u_0,\ldots,u_p$. What is the permutation $S_\lambda^{(8)}$ induces on $u_0,\ldots,u_p$?

d) Analyze the permutation that T_λ induces on the functions $\lambda_0,\ldots,\lambda_p$ and on the functions $u_0,\ldots,u_p$. Identify $\lambda_p(T_\lambda)$ and $\lambda_p(T_\lambda^{-1})$ in particular.

2. Prove Theorem 4.9.
Hint: Use Theorem 4.7 and Exercise 1. Consider how $W_p(v^8,u^8)$ splits over $\mathbb{Q}(u)$. (Note that u is invariant with respect to group generated by $S_\lambda^{(8)}$ and T_λ.)

3. Prove the "octicity" of the u–v modular equation. That is, for $p\equiv\pm1$ mod 8 the nonzero entries of the table associated with Ω_p lie only on the main diagonal and every eighth sub and super diagonal, while for $p\equiv\pm3 \bmod 8$ the nonzero entries are only in every second entry of every fourth diagonal.

4. a) Prove the symmetries (or antisymmetries) of the u–v modular equation with respect to reflection through both diagonals.
b) Evaluate the row sums explicitly from Theorem 4.9.
c) Observe that with the aid of the "octicity" one can read off the modular equations of degrees 3, 5, and 7. Verify the modular equations of degrees 11 and 13. This requires either calculating the u_i at a single value of q, or using Exercise 6.

5. Show that Ω_7 can be written as

$$(1-u^8)(1-v^8)=(1-uv)^8 \tag{4.5.3}$$

or as

$$(kl)^{1/4}+(k'l')^{1/4}=1\,. \tag{4.5.4}$$

6. From our analysis we know that

$$\Omega_p(v,u)=v^{p+1}+\sum_{k,j=1}^{p}c_{k,j}u^kv^j+(-1)^{(p^2-1)/8}u^{p+1}\,.$$

a) Show that $c_{1,1}=-(-1)^{(p^2-1)/8}2^{(p-1)/2}$
Hint: $\Omega(u_0,u)=0$ and $u=\sqrt{2}q^{1/8}+O(u^2)$ while $u_0=\sqrt{2}q^{1/8p}+O(u_0^2)$. Thus

$$0=(-1)^{(p^2-1)/8}u^p+c_{1,1}u_0+O(u_0u)$$

and

$$c_{1,1}=-(-1)^{(p^2-1)/8}\lim_{u\to0}\frac{u^p}{u_0}\,.$$

b) Show that if $0<u<v<1$ and $\Omega(v,u)=0$, then

$$v^p\le 2^{(p-1)/2}u \qquad\text{and}\qquad \lim_{u\to0}\frac{v^p}{u}=2^{(p-1)/2}\,.$$

c) Hence if $W_p(\gamma_n,\gamma_{n+1})=0$ with $1>\gamma_n>\gamma_{n+1}>0$, one has

$$\gamma_{n+1}\ge\frac{\gamma_n^p}{4^{p-1}} \qquad\text{and}\qquad \lim_{n\to\infty}\frac{\gamma_n^p}{\gamma_{n+1}}=4^{p-1}\,.$$

7. In 1858, Hermite and Kronecker separately gave solutions of a general quintic using quintic modular equations. Hermite's method is outlined below.

a) Let

$$\Phi_i:=(u_5-u_i)(u_{i+1}-u_{i-1})(u_{i+2}-u_{i-2})\qquad i=0,1,\ldots,4$$

where $i+j$ is chosen mod 5. Then

$$\left(\frac{1}{2^45^3}\right)^{1/4}\frac{1}{u(1-u^8)^{1/2}}\,\Phi_i \qquad i=0,\ldots,4$$

are the five roots of the quintic

$$x^5-x-\frac{2}{5^{5/4}}\,\frac{1+u^8}{u^2(1-u^8)^{1/2}}\,.$$

b) The quintic modular equation (4.1.21)

$$u^6-v^6+5u^2v^2(u^2-v^2)+4uv(1-u^4v^4)=0$$

can equivalently be transformed into

$$x^5 - 2^4 5^3 u^4 (1-u^8)^2 x - 2^6 5^{5/2} u^3 (1-u^8)^2 (1+u^8) = 0 .$$

The details are formidable.

c) Any quintic can be algebraically reduced (via solution of a quartic equation) to the *Bring form*

$$x^5 - x - a$$

and hence a) and c) provide a solution of the quintic in terms of the roots of the modular equation. This requires solving

$$a = \frac{2}{5^{5/4}} \frac{1+u^8}{u^2(1-u^8)^{1/2}}$$

and leads to a quartic equation in u^4.

The amount of calculation required above is prohibitive. However, that some combination of the u_i solves a quintic is not overly surprising since the Galois group of the quintic modular equation (4.1.21) is A_5. The reduction to Bring form in c) is effected via the Tschirnhaus substitution.

8. (*On the Galois groups for W_5 and W_7 over $\mathbb{Q}(\lambda)$*)

a) For $p = 5$, S_λ and T_λ induce the following permutations of the roots $(i = \lambda_i)$

$$S_\lambda\colon\ (0,1,2,3,4,5) \to (1,2,3,4,0,5)$$
$$T_\lambda\colon\ (0,1,2,3,4,5) \to (0,5,3,1,2,4) .$$

b) For $p = 7$

$$S_\lambda\colon\ (0,1,2,3,4,5,6,7) \to (1,2,3,4,5,6,0,7)$$
$$T_\lambda\colon\ (0,1,2,3,4,5,6,7) \to (0,3,1,4,6,7,5,2) .$$

c) Show, using a), that the Galois group of W_5 contains A_5 and is not solvable.

d) Show, using b), that the Galois group for W_7 is not solvable.

In both cases these permutations actually generate the Galois group. (See Exercise 10 of 4.4, and Exercise 1 of 4.5.)

4.6 *THE MULTIPLIER*

As we saw in Section 4.4, the pth-order transformation can be considered as determined by $k := k(q)$ and $l := k(q^{1/p})$. We define M_p, the *multiplier of order p*, by

$$\text{(4.6.1)} \qquad M_p(l,k) := \frac{\theta_3^2(q)}{\theta_3^2(q^{1/p})} = \frac{K(k)}{K(l)}$$

and in the future will denote $K(l) := L$.

Theorem 4.10

If $K := k(q)$ and $l := k(q^{1/p})$, then $W_p(l,k) = 0$ and

$$\text{(4.6.2)} \qquad pM_p^2 = \frac{ll'^2}{kk'^2}\frac{dk}{dl} = \frac{v(1-v^8)}{u(1-u^8)}\frac{du}{dv} .$$

In particular, M_p is an algebraic function of k and l.

Proof. Since $\pi K'/K = -\log q$ [by Theorem 2.3(*b*)], we have

$$\text{(4.6.3}a\text{)} \qquad \frac{d}{dk}\left(\frac{K'}{K}\right) = -\frac{1}{2}\frac{\pi}{kk'^2K^2}$$

on using (2.3.10). Similarly,

$$\text{(4.6.3}b\text{)} \qquad \frac{d}{dl}\left(\frac{L'}{L}\right) = -\frac{1}{2}\frac{\pi}{ll'^2L^2} .$$

Now as $pL'/L = K'/K$ [again by Theorem 2.3(*b*)], we can write the l, k form of (4.6.2) on dividing (4.6.3*a*) by (4.6.3*b*). We now verify the u–v form directly. □

When M_p is given by $v(1-v^8)/[u(1-u^8)]\,(du/dv)$ as a function of u and v, we write $M_p(v,u)$. In this form we see that M_p^2 is rational. In fact $M_p(v,u)$ is rational. (See also Exercise 1.)

Let us use (4.6.2) to compute M_2 and M_3. When $p := 2$, we have $l = 2\sqrt{k}/(1+k)$ and $k = (1-l')/(1+l')$, by equation (2.1.15). Thus

$$\text{(4.6.4)} \qquad 2M_2^2 = \frac{ll'^2}{kk'^2}\frac{dk}{dl} = \frac{ll'^2}{kk'^2}\frac{\sqrt{k}(1+k)^2}{1-k} = \frac{2}{(1+k)^2}$$

and

$$M_2(l,k) = \frac{1}{1+k} = \frac{1+l'}{2}$$

which corresponds with Theorem 2.6.

When $p:=3$, we have $\sqrt{lk}+\sqrt{l'k'}=1$, by equation (4.2.6). This produces, on differentiating implicitly and using (4.6.2),

$$3M_3^2=-\frac{l'^2\sqrt{lk}-l^2\sqrt{l'k'}}{k'^2\sqrt{lk}-k^2\sqrt{l'k'}}=-\frac{\sqrt{lk}-l^2}{\sqrt{lk}-k^2}=-\frac{1-\sqrt{l^3/k}}{1-\sqrt{k^3/l}}\,.$$

Let $\alpha^4:=k^3/l$. Then $l^3/k=[(2+\alpha)/(1+2\alpha)]^4$ and

(4.6.5) $$3M_3^2=\frac{3}{(2\alpha+1)^2}\qquad\text{or}\qquad M_3=\frac{1}{2\alpha+1}\,.$$

(See Exercise 2 of Section 4.1.) But $\alpha=u^3/v$ so that

$$M_3=\frac{v}{v+2u^3}=\frac{2v^3-u}{3u}$$

because

$$\frac{3}{2\alpha+1}=2\left(\frac{2+\alpha}{2\alpha+1}\right)-1\,.$$

For $p:=5$ or 7, similar, but more elaborate, calculation produces

(4.6.6) $$M_5=\frac{u+v^5}{5u(1+u^3v)}=\frac{v(1-uv^3)}{v-u^5}$$

(4.6.7) $$M_7=\frac{v(1-uv)[1-uv+(uv)^2]}{v-u^7}=-\frac{u-v^7}{7u(1-uv)[1-uv+(uv)^2]}\,.$$

(See Cayley [1895].) Many other multipliers have been calculated and can be found in Ramanujan's collected works, Cayley [1874], Tannery and Molk [1893], Weber [08] and elswhere. The main technique for larger p is via manipulation of theta series. Thus one has Ramanujan's form of the multiplier for 13:

(4.6.8)
$$13M_{13}(l,k)=\left(\frac{l}{k}\right)^{1/2}+\left(\frac{l'}{k'}\right)^{1/2}-\left(\frac{ll'}{kk'}\right)^{1/2}-4\left(\frac{ll'}{kk'}\right)^{1/3}=\frac{1}{M_{13}(k,l)}\,.$$

We list also

(4.6.9) $$17M_{17}(l,k)=\left(\frac{l}{k}\right)^{1/2}+\left(\frac{l'}{k'}\right)^{1/2}+\left(\frac{ll'}{kk'}\right)^{1/2}-2\left(\frac{ll'}{kk'}\right)^{1/4}\left[1+\left(\frac{l}{k}\right)^{1/4}+\left(\frac{l'}{k'}\right)^{1/4}\right]=\frac{1}{M_{17}(k,l)}\,.$$

We conclude this section by touching on the matter of *singular values*, k_p, which for us are defined to be the solutions in $(0,1)$ of $W_p(k',k)=0$. These are often called *singular moduli* for the function λ. Corresponding values for J are discussed in Exercise 6.

Then, since $K'(k)/K(k)$ is isotone, Theorem 2.3(*b*) shows that this is the unique solution to

$$\frac{K'}{K}(k_p)=\sqrt{p}\qquad 0<k_p<1\,.$$

In the notation of equation (3.2.1), $k_p=\lambda^*(p)$ and $k_p'=\lambda^*(1/p)$, so that $k_p=k(e^{-\pi\sqrt{p}})$ and $l_p:=k_p'=k(e^{-\pi/\sqrt{p}})$. Sophisticated number-theoretic techniques are available for computing k_p for large p, without knowledge of W_p. This is discussed briefly in Exercise 5. For small p one can solve directly for k_p. Thus

$$\begin{array}{lll}
k_1=\dfrac{1}{\sqrt{2}} & l_1=\dfrac{1}{\sqrt{2}} & 2k_1l_1=1\\
k_2=\sqrt{2}-1 & l_2=\sqrt{2\sqrt{2}-2} & \\
k_3=\dfrac{\sqrt{2}(\sqrt{3}-1)}{4} & l_3=\dfrac{\sqrt{2}(\sqrt{3}+1)}{4} & 2k_3l_3=\dfrac{1}{2}\\
k_4=3-2\sqrt{2} & l_4=2^{1/4}(2\sqrt{2}-2) & \\
k_5=\dfrac{\sqrt{\sqrt{5}-1}-\sqrt{3-\sqrt{5}}}{2} & l_5=\dfrac{\sqrt{\sqrt{5}-1}+\sqrt{3-\sqrt{5}}}{2} & 2k_5l_5=\sqrt{5}-2\\
k_7=\dfrac{\sqrt{2}(3-\sqrt{7})}{8} & l_7=\dfrac{\sqrt{2}(3+\sqrt{7})}{8} & 2k_7l_7=\dfrac{1}{8}\\
k_9=\dfrac{(\sqrt{2}-3^{1/4})(\sqrt{3}-1)}{2} & l_9=\dfrac{(\sqrt{2}+3^{1/4})(\sqrt{3}-1)}{2} & 2k_9l_9=(2-\sqrt{3})^2\,.
\end{array}$$

(4.6.10)

A more comprehensive list is given in the next chapter. A profusion of modular equations of degrees 3, 5, and 7 are given in Chapter 19 of Ramanujan's Second Notebook.

Comments and Exercises

1. From the results of Section 1.5 (in particular Theorem 1.5 and Exercise 1) we know that $G(k):=k^{1/2}k'K(k)$ satisfies

$$G(k)=\sqrt{c\,\frac{dk}{dl}}\,G(l)$$

where k and l are solutions of the pth-order modular equation W_p. Use this to show that

$$M_p^2(l, k) := \left[\frac{K(l)}{K(k)}\right]^2 = c\,\frac{ll'^2}{kk'^2}\,\frac{dk}{dl}$$

where c is a constant. This provides an easy alternate derivation of Theorem 4.10 up to the evaluation of the constant c.

2. a) Verify the computation of M_3 in (4.6.5).
b) Compute M_5 in (4.6.6).

Cayley [1874] discusses algebraic methods for computing W_p and M_p at length. These seem only to be entirely reasonable for 2, 3, 5, 7, and in part, 11. The discussion therein also illuminates the rational nature of $M_p(u, v)$.

3. a) Show that $pM_p(l, k)M_p(k', l') = 1$.
b) Use Theorem 4.10 to show that for all u and v,

$$[pM_p(v, u)M_p((-1)^{(p^2-1)/8}u, v)]^2 = 1\,.$$

Hint: Consider the similar symmetry of Ω_p.

4. a) Cayley observes that given any polynomial identity $F(u, v) = 0$ which satisfies $F(u, v) = F(-u, -v)$, one can produce a similar identity $G(u^2, v^2) = 0$, with G of the same degree. One uses

$$(4.6.11)\qquad [F(u, v)F(u, -v)F(-u, v)F(-u, -v)]^{1/2} = 0\,.$$

b) Use this technique to develop modular equations and multipliers in terms of the u^{2n}, v^{2n} $(n := 1, 2, 4)$ for $p := 2, 3, 5, 7$. (See Cayley [1874].)

5. Verify the singular values in (4.6.10). In each odd case one verifies $t_n = 2k_nk_n'$ first and uses

$$k_n = (\sqrt{1+t_n} - \sqrt{1-t_n})/2$$
$$l_n = (\sqrt{1+t_n} + \sqrt{1-t_n})/2\,.$$

The invariants of (3.2.9) to (3.2.13) lie at the heart of calculating singular values. Armed with these and either Ramanujan's insight or some knowledge of group theory, singular values can be calculated in profusion. Watson, in a long series of papers commencing with Watson [32], has recreated what he believes to be Ramanujan's procedure, while Weber [08] explains the classical theory and lists many examples. Zucker [77] indicates an attractive way of calculating many large singular values such as Ramanujan's celebrated

$$(4.6.12)\quad k_{210} = (\sqrt{2}-1)^2(2-\sqrt{3})(\sqrt{7}-\sqrt{6})^2(8-3\sqrt{7}) \times(\sqrt{10}-3)^2(4-\sqrt{15})^2(\sqrt{15}-\sqrt{14})(6-\sqrt{35})\,.$$

Zucker's methods are described in Section 9.2.

6. In this exercise we sketch the relationship between binary quadratic forms and *singular invariants or values* for F_p [solutions of $F_p(j, j) = 0$].

a) Let

$$S := \begin{pmatrix} a & b \\ c & d \end{pmatrix}$$

where $|S| = ad - bc = p > 0$ and a, b, c, d are integral, and assume with no loss of generality that $c > 0$, $b \neq 0$. We say t with $\mathrm{im}(t) > 0$ *satisfies complex multiplication* by μ if $(\mu t, \mu) = S(t, 1)$ so that $t = (at + b)/(ct + d)$. In particular, t is the solution with $\mathrm{im}(t) > 0$ to an integral equation $Ax^2 + Bx + C = 0$ with $-D := B^2 - 4AC < 0$.

[This corresponds to asking for which μ one can solve $\wp(\mu z, w_1, w_2) = R(\wp(z, w_1, w_2))$ for some rational function R. Here $\wp(z) := \wp(z, w_1, w_2)$ is the Weierstrass $\wp$ function of Section 1.7. Or, in other words, for which μ does the lattice L generated by w_1 and w_2 contain the lattice μL? Hence, the multiplication.]

b) Suppose that

$$t = \frac{at+b}{ct+d} \qquad \text{and} \qquad t^* = \frac{a^*t+b^*}{c^*t+d^*}$$
$$(4.6.13)\qquad ad - bc = p\,,\quad a^*d^* - b^*c^* = 1\,.$$

Then $j(t^*) = j(t)$. Also t^* solves a quadratic with the same discriminant as that for t, and t^* possesses a multiplication by μ if and only if t does. Now (4.4.6) implies $F_p(x, j) = 0$ is solved by $j(t)$, because $S \equiv A_i \bmod \Gamma$ for some i and hence $j(t) = j_i(t)$. Thus $F_p(j, j) = 0$ is solved by $j(t)$ exactly when t possesses complex multiplication. Note that $F_p(j, j)$ will have lower degree than $F_p(x, j)$.

c) Since j is one to one on the fundamental region, $j(t) = j(t^*)$ if and only if the associated primitive binary quadratic forms are properly equivalent. A binary form $ax^2 + bxy + cy^2 = 0$ is *primitive* if $\gcd(a, b, c) = 1$. Two forms are *properly equivalent* if there is an integral linear transformation of determinant 1 converting the one into the other. (See Dickson [71, vol. 3].)

d) Thus the study of the degree of $F_p(j, j)$ becomes the study of $h(-D)$: the *class number* of primitive forms of negative discriminant $-D$. More of this is sketched in Hardy [40, chap. 10], and in Tannery and Molk [1893].

7. For fixed m and p let $\gamma_0 := k_m$ be the mth singular value and let γ_n be the sequence of solutions of $W_p(\gamma_n, \gamma_{n+1}) = 0$ as defined in Exercise 6 of Section 4.5. Use Theorem 2.3 and (3.2.3) to show that

$$e^{\pi\sqrt{m}/2} = \lim_{n\to\infty} \left(\frac{4}{\gamma_n}\right)^{1/p^n}.$$

This provides an algorithm of order p for computing $e^{-\pi\sqrt{m}}$. When $p := 2$, this reduces to the algorithm in Exercise 3 of Section 2.5.

By the same process as in Section 4.5 one can produce polynomials in $x := M_p^{-1}(l, k)$ and k. Cayley [1874], following Joubert, gives

$$x^4 - 6x^2 + 8(1-2k^2)x - 3 = 9 \qquad p := 3 \tag{4.6.14}$$

$$x^6 - 10x^5 + 35x^4 - 60x^3 + 55x^2 + [64(2kk')^2 - 26]x + 5 = 0 \qquad p := 5 \tag{4.6.15}$$

and

$$\begin{aligned} &x^8 - 28x^6 + 112(1-2x^2)x^5 - 210x^4 \\ &+ 224(1-2k^2)x^3 - [140 + 1344(2kk')^2]x^2 \\ &+ [48 + 512(2kk')^2](1-2k^2)x + 7 = 0 \qquad p := 7. \end{aligned} \tag{4.6.16}$$

He gives a similar expression when $p := 11$.

8. a) Verify (4.6.14) and observe that $3M_3(1/\sqrt{2}, k_9) = \sqrt{3 + 2\sqrt{3}}$.
b) Explicitly solve (4.6.14) to produce M_3^{-1} as a function of k.
c) Use (4.6.15) to determine k_5.

4.7 *CUBIC MODULAR IDENTITIES*

Ramanujan in his notebooks gives the following remarkable identity:

$$\frac{\theta_3(q)}{\theta_3(q^9)} - 1 = \left[\frac{\theta_3^4(q^3)}{\theta_3^4(q^9)} - 1\right]^{1/3}. \tag{4.7.1}$$

[See (24.28) and (24.29) of Chapter 18 of his second notebook in Berndt [Pr].]

An equivalent form and some variants of this formula are established in the next theorem.

Theorem 4.11

With

$$k := \frac{\theta_2^2(q)}{\theta_3^2(q)} \qquad \gamma := \frac{\theta_2^2(q^3)}{\theta_3^2(q^3)}$$

one has

(*a*) $$\left[3\frac{\theta_3(q^9)}{\theta_3(q)} - 1\right]^3 = 4\left(\frac{k^3k'^3}{\gamma\gamma'}\right)^{1/4} = 9\frac{\theta_3^4(q^3)}{\theta_3^4(q)} - 1$$

(*b*) $$\left[3\frac{\theta_4(q^9)}{\theta_4(q)} - 1\right]^3 = 4\left(\frac{k^3/k'^6}{\gamma/\gamma'^2}\right)^{1/4} = 9\frac{\theta_4^4(q^3)}{\theta_4^4(q)} - 1$$

(*c*) $$\left[3\frac{\theta_2(q^9)}{\theta_2(q)} - 1\right]^3 = -4\left(\frac{k'^3/k^6}{\gamma'/\gamma^2}\right)^{1/4} = 9\frac{\theta_2^4(q^3)}{\theta_2^4(q)} - 1.$$

Proof. We establish only (*a*). Then (*b*) and (*c*) follow (Exercise 2). It is most convenient to use the quintuple-product extension of Jacobi's triple product, which is developed in Section 9.4. Equation (9.4.3) with $j := 6$ and $k := 1$ may be remanipulated to show that

$$3\theta_3(q^9) - \theta_3(q) = 2\prod_{n=1}^{\infty}(1-q^n)(1+q^{2n})(1+q^{6n-3}).$$

Hence, with (3.1.6),

$$\theta_3(q)[3\theta_3(q^9) - \theta_3(q)]^3 = 8\prod_{n=0}^{\infty}(1+q^{6n+3})^3$$

$$\prod_{n=1}^{\infty}(1-q^{2n})^4(1-q^{2n-1})^3 \quad (1+q^{2n})^3(1+q^{2n-1})^2$$

and Euler's identity (3.1.4) reduces this to

$$8\prod_{n=0}^{\infty}(1+q^{6n+3})^3\prod_{n=0}^{\infty}(1+q^{2n+1})^3\prod_{n=1}^{\infty}\left(\frac{1-q^{2n}}{1+q^{2n-1}}\right)^4.$$

Now (3.2.9*iv*) shows

$$\prod_{n=0}^{\infty}(1+q^{2n+1})^3 = \sqrt{2}q^{1/8}(kk')^{-1/4}$$

and

$$\prod_{n=0}^{\infty}(1+q^{6n+3})^3 = \sqrt{2}q^{3/8}(\gamma\gamma')^{-1/4}$$

while (3.1.4), (3.1.7), and (3.1.8) combine to yield

$$\prod_{n=1}^{\infty}\left(\frac{1-q^{2n}}{1+q^{2n-1}}\right)^4 = \frac{1}{4}q^{-1/2}\theta_2^2(q)\theta_4^2(q).$$

These identities result in

$$\theta_3(q)[3\theta_3(q^9)-\theta_3(q)]^3 = 4\,\frac{\theta_2^2\theta_4^2}{(kk')^{1/4}(\gamma\gamma')^{1/4}} = 4\theta_3^4\,\frac{(kk')^{3/4}}{(\gamma\gamma')^{1/4}}\,. \tag{4.7.2}$$

This establishes the first equality for part (*a*). The second is most easily seen by using equation (4.1.15), with $\gamma := k$ and $k := l$, to write $k^3/\gamma = [(2+\alpha)/(2\alpha+1)]^4$, $k'^3/\gamma' = [(1-\alpha)/(2\alpha+1)]^4$, and using (4.1.19) or (4.6.5) to write $\theta_3^4(q^3)/\theta_3^4(q) = 1/(2\alpha+1)^2$. Then both sides of the second equality become $4(2+\alpha)(1-\alpha)/(2\alpha+1)^2$. □

These identities have many remarkable consequences some of which we leave as exercises. Two, however, are worthy of more explicit analysis.

AN ITERATION FOR THE CUBIC MULTIPLIER. In decreasing form, as above, we consider the multiplier $M_n := K_{n+1}/K_n$ where $K_n := K(q^{3^n})$. Then part a) of Theorem 4.11 shows that, with $m_n := 3M_n$, we have

$$m_{n+1} = \frac{[(m_n^2-1)^{1/3}+1]^2}{m_n} \tag{4.7.3}$$

where

$$m_0 = \left[1+2\sqrt{2}\,\frac{(2kk')^{3/4}}{(2\gamma\gamma')^{1/4}}\right]^{1/2}. \tag{4.7.4}$$

Alternatively, part (*b*) shows that if we set $r_n := 3\theta_4^2(q^{3^{n+1}})/\theta_4^2(q^{3^n})$, so that $m_n = (r_n+3)/(r_n-1)$ (see Exercise 8). We have

$$r_{n+1} = \frac{[(r_n^2-1)^{1/3}+1]^2}{r_n} \tag{4.7.5}$$

where

$$r_0 = \left[1+2\sqrt{2}\,\frac{(2k/k'^2)^{3/4}}{(2\gamma/\gamma'^2)^{1/4}}\right]^{1/2}. \tag{4.7.6}$$

This latter is more suitable when we begin with an even singular value. We have written (4.7.4) and (4.7.5) in a form consistent with Ramanujan's invariants G_n and g_n. [See (3.2.13) and Exercise 5, Section 3.2.] In these terms, the iterations are initialized by

$$m_0 := m(n) := [1+(\sqrt{2}G_{9n}/G_n^3)^3]^{1/2} \tag{4.7.7}$$

and $\qquad q := e^{-\pi\sqrt{n}}$

$$r_0 := r(n) := [1+(\sqrt{2}g_{9n}/g_n^3)^3]^{1/2}\,. \tag{4.7.8}$$

We also write $M(n) := m(n)/3$.

CUBIC RECURSIONS FOR G_n AND g_n. We have

$$9\,\frac{\theta_3^4(q^3)}{\theta_3^4(q)} = 1+2\sqrt{2}\,\frac{G_{9n}^3}{G_n^9}$$

and, using the theta inversion formula in part (*a*),

$$\frac{\theta_3^4(q)}{\theta_3^4(q^3)} = 1+2\sqrt{2}\,\frac{G_n^3}{G_{9n}^9}\,.$$

Thus

$$9 = \left(1+2\sqrt{2}\,\frac{G_{9n}^3}{G_n^9}\right)\left(1+2\sqrt{2}\,\frac{G_n^3}{G_{9n}^9}\right). \tag{4.7.9}$$

Similarly

$$9 = \left(1+2\sqrt{2}\,\frac{g_{9n}^3}{g_n^9}\right)\left(1-2\sqrt{2}\,\frac{g_n^3}{g_{9n}^9}\right). \tag{4.7.10}$$

Thus given G_n or g_n, we have a simple equation to solve for G_{9n} or g_{9n}. For example, with $n := \frac{1}{3}$ we have $G_3 = G_{1/3}$, and with $x := G_3$ we know that $(1+2\sqrt{2}x^{-6})^2 = 9$ or $G_3 = 2^{1/12}$. Similarly, $g_{2/3}^{-1} = g_6$ so that (4.7.10) yields $g_6^{12} - g_6^{-12} = 4\sqrt{2}$ and $g_6^6 = \sqrt{2}+1$.

A more tractable recursion can be attained by observing that

$$3\,\frac{\theta_3(q^9)}{\theta_3(q)} - 1 = \sqrt{2}\,\frac{G_{9n}}{G_n^3}$$

and

$$\frac{\theta_3(q)}{\theta_3(q^9)} - 1 = \sqrt{2}\,\frac{G_{9n}}{G_{81n}^3}\,.$$

Thus

$$3 = \left(\sqrt{2}\,\frac{G_{9n}}{G_{81n}^3}+1\right)\left(\sqrt{2}\,\frac{G_{9n}}{G_n^3}+1\right) \tag{4.7.11}$$

and, rearranging,

$$G_{81n}^3 = G_{9n}\,\frac{\sqrt{2}G_{9n}+G_n^3}{\sqrt{2}G_n^3-G_{9n}}\,. \tag{4.7.12}$$

Correspondingly

$$g_{81n}^3 = g_{9n}\frac{g_n^3+\sqrt{2}g_{9n}}{g_{9n}-\sqrt{2}g_n^3}. \tag{4.7.13}$$

From these two formulae, and other singular values given by Ramanujan, one can give explicit equations for some very large invariants (G_{2025}^3, G_{2997}^3, g_{4698}^3, for example). We illustrate with g_{4698}. Ramanujan gives

$$g_{58}^2 = \frac{5+\sqrt{29}}{2}$$

$$g_{522} = \left(\frac{5+\sqrt{29}}{2}\right)^{1/2}(5\sqrt{29}+11\sqrt{6})^{1/6}\left(\sqrt{\frac{9+3\sqrt{6}}{4}}+\sqrt{\frac{5+3\sqrt{6}}{4}}\right).$$

Then manipulation of (4.7.13) yields

$$g_{4698}^3 =$$

$$\left(\frac{\sqrt{29}-5}{2}\right)^{1/2}\frac{(\sqrt{29}+5)+\sqrt{2}(11\sqrt{6}+5\sqrt{29})^{1/6}(\sqrt{9+3\sqrt{6}}+\sqrt{5+3\sqrt{6}})}{(\sqrt{29}-5)-\sqrt{2}(11\sqrt{6}-5\sqrt{29})^{1/6}(\sqrt{9+3\sqrt{6}}-\sqrt{5+3\sqrt{6}})}.$$

(See also Exercise 13.) Analogous results for quintic and septic multipliers are treated in Section 9.5.

Comments and Exercises

The quintuple-product identity was certainly known in essence to Ramanujan so that our derivation of Theorem 4.11 is in all likelihood similar to that which he had in mind. The proof we give in Section 9.4 is self-contained and can be read with ease now. Biagioli [Pr] has given a modular function proof of (4.7.1).

1. a) Show that (4.7.1) is equivalent to

$$3\frac{\theta_3(q^9)}{\theta_3(q)}-1=\left[\frac{9\theta_3^4(q^3)}{\theta_3^4(q)}-1\right]^{1/3}$$

(either by modular considerations or by direct inversion of the underlying quartic polynomial).

b) Show that the AGM iterations in theta form can be written as

$$\frac{\theta_3(q)}{\theta_3(q^4)}-1=\left[\frac{\theta_3^2(q^2)}{\theta_3^2(q^4)}-1\right]^{1/2}$$

or as

$$2\frac{\theta_3(q^4)}{\theta_3(q)}-1=\left[2\frac{\theta_3^2(q^2)}{\theta_3^2(q)}-1\right]^{1/2}.$$

(Note that in this case the replacement of q by $-q$ does not give a formula in θ_4.)

2. a) Show that Theorem 4.11, parts (*b*) and (*c*) are equivalent to part (*a*).

b) Derive part (*c*) directly from (9.4.3).

3. Use (4.7.9) and (4.7.10) to verify that

i) $G_9^3 = (\sqrt{3}+1)/\sqrt{2}$

ii) $g_{18}^3 = \sqrt{3}+\sqrt{2}$

iii) $G_{27}^3 = 2^{1/4}/(2^{1/3}-1)$.

4. a) Use Exercise 3 and (4.7.12) and (4.7.13) to verify that

i) $G_{81}^3 = \dfrac{(2\sqrt{3}+2)^{1/3}+1}{(2\sqrt{3}-2)^{1/3}-1}$

ii) $g_{162}^3 = \dfrac{1+(2\sqrt{6}+4)^{1/3}}{1-(2\sqrt{6}-4)^{1/3}}$.

b) Calculate G_{243} and g_{54}.

5. Show that, in the notation of Proposition 3.1,

a) $\prod_{j=2}^{4}[\theta_j(q)-3\theta_j(q^9)] = 4\theta_1^+(q)$

b) $\prod_{j=2}^{4}[\theta_j(q^9)-\theta_j(q)] = 4\theta_1^+(q^9)$.

6. Show that

$$\theta_2(q^9)[\theta_2(q)-\theta_2(q^9)]^3+\theta_4(q^9)[\theta_4(q)-\theta_4(q^9)]^3 = \theta_3(q^9)[\theta_3(q)-\theta_3(q^9)]^3.$$

7. Use Schlafli's equation (Exercise 6 of Section 4.1) to establish that

i) $G_5^4 = \dfrac{\sqrt{5}+1}{2}$

ii) $g_{10}^2 = \dfrac{\sqrt{5}+1}{2}$

iii) $G_{25} = \dfrac{\sqrt{5}+1}{2}$.

8. In the notation of (4.7.7) and (4.7.8) show using (4.1.15) that

i) $[m(n)-1][r(n)-1]=4$

and

ii) $r(4n)=\sqrt{m(n)+r(n)+3}=\sqrt{r(n)m(n)}$.

Also (4.7.9) gives

iii) $m\left(\frac{1}{n}\right)=M^{-1}\left(\frac{n}{9}\right)=3m^{-1}\left(\frac{n}{9}\right).$

9. a) Given that

$$G_{21}^{-6}=\left(\frac{3-\sqrt{7}}{\sqrt{2}}\right)\left(\frac{\sqrt{7}-\sqrt{3}}{2}\right)^{3/2}$$

verify that

$$G_{7/3}^{-6}=\left(\frac{3-\sqrt{7}}{\sqrt{2}}\right)\left(\frac{\sqrt{7}+\sqrt{3}}{2}\right)^{3/2} \quad \text{and}$$

$$M^{-1}\left(\frac{7}{3}\right)=\sqrt{3}\left(\frac{\sqrt{3}+1}{\sqrt{2}}\right)\sqrt{2\sqrt{7}-3\sqrt{3}}\,.$$

b) Use the modular equations of degrees 3 and 7 to verify the value of G_{21}.

10. In each case, given the first invariant verify the following ones.

a) $G_{33}^{-6}=\left(\frac{\sqrt{11}-3}{\sqrt{2}}\right)\left(\frac{\sqrt{3}-1}{\sqrt{2}}\right)^{3}$, $G_{11/3}^{-6}=\left(\frac{\sqrt{11}+3}{\sqrt{2}}\right)\left(\frac{\sqrt{3}-1}{\sqrt{2}}\right)^{3}$ and

$$M^{-1}\left(\frac{11}{3}\right)=\sqrt{3}\sqrt{2\sqrt{3}+\sqrt{11}}\left(\frac{\sqrt{11}-3}{\sqrt{2}}\right).$$

b) $G_{57}^{-6}=\left(\frac{3\sqrt{19}-13}{\sqrt{2}}\right)\left(\frac{\sqrt{3}-1}{\sqrt{2}}\right)^{3}$, $G_{19/3}^{-6}=\left(\frac{3\sqrt{19}-13}{\sqrt{2}}\right)\left(\frac{\sqrt{3}+1}{\sqrt{2}}\right)^{3}$

and

$$M^{-1}\left(\frac{19}{3}\right)=\sqrt{3}\sqrt{2\sqrt{19}+5\sqrt{3}}\left(\frac{\sqrt{3}-1}{\sqrt{2}}\right)^{3}.$$

c) $G_{93}^{-6}=\left(\frac{39-7\sqrt{31}}{\sqrt{2}}\right)\left(\frac{\sqrt{31}-3\sqrt{3}}{2}\right)^{3/2}$,

$G_{31/3}^{-6}=\left(\frac{39-7\sqrt{31}}{\sqrt{2}}\right)\left(\frac{\sqrt{31}+3\sqrt{3}}{2}\right)^{3/2}$ and

$$M^{-1}\left(\frac{31}{3}\right)=\sqrt{3}\left(\frac{\sqrt{31}-3\sqrt{3}}{2}\right)^{3/2}\left(\frac{\sqrt{3}+1}{\sqrt{2}}\right)^{3}.$$

d) $g_{78}^{-6}=(\sqrt{26}-5)\left(\frac{\sqrt{13}-3}{2}\right)^{3}$, $g_{26/3}^{-6}=(\sqrt{26}+5)\left(\frac{\sqrt{13}-3}{2}\right)^{3}$ and

$$r\left(\frac{26}{3}\right)=\sqrt{3}\left(\frac{\sqrt{13}-3}{2}\right)^{3/2}\sqrt{6+34\sqrt{2}+15\sqrt{13}}.$$

e) $g_{30}^{-6}=(\sqrt{10}-3)(\sqrt{5}-2)$, $g_{10/3}^{-6}=(\sqrt{10}-3)(\sqrt{5}+2)$ and

$$r\left(\frac{10}{3}\right)=\sqrt{3}(\sqrt{2}-1)(\sqrt{5}+2).$$

11. a) Verify that $m(\frac{1}{3})=\sqrt{3}$ and $r(\frac{2}{3})=\sqrt{6}+\sqrt{3}$.
b) Hence verify that $m(\frac{2}{3})=3\sqrt{2}+2\sqrt{3}-\sqrt{6}-3$ and that $r(\frac{8}{3})=\sqrt{3(\sqrt{3}+\sqrt{2})}$.
c) Verify that $m(1)=\sqrt{3+\sqrt{12}}$ and $r(4)=\sqrt{3+\sqrt{3}+\sqrt{9+6\sqrt{3}}}$.
d) Verify that $r(2)=\sqrt{2}+\sqrt{3}$ and $m(\frac{1}{2})=\sqrt{6}-\sqrt{2}+1$. Hence $m(\frac{1}{18})=3(3\sqrt{6}+7-4\sqrt{3}-5\sqrt{2})$.
e) Verify that $m(\frac{1}{6})=(3-\sqrt{6})(\sqrt{2}+1)$ and $m(\frac{1}{12})=(6\sqrt{3}+9)-(4\sqrt{6}+6\sqrt{2})$.

12. a) Show that (4.7.9) can be written as

$$\left(\frac{x}{y}\right)^{2}+\left(\frac{y}{x}\right)^{2}=2\sqrt{2}[(xy)-(xy)^{-1}]$$

where $x:=G_N^3$ and $y:=G_{9N}^3$. Hence compute G_3 and G_9.
b) Find the parallel expression for g_N^3, g_{9N}^3. [Compare (4.1.27).]

13. One can explicitly solve (4.7.9) and (4.7.10) to obtain the following formulae.

a) Show that G_{9N}^3 and $G_{N/9}^3$ are the two solutions to

$$x^2-\sqrt{2}G_N[G_N^8+\sqrt{G_N^{16}+G_N^8+1}]x+G_N^2[G_N^8+1+\sqrt{G_N^{16}+G_N^8+1}]=0\,.$$

b) Show that g_{9N}^3 and $-g_{N/9}^3$ are the two solutions to

$$x^2-\sqrt{2}g_N[g_N^8+\sqrt{g_N^{16}-g_N^8+1}]x-g_N^2[g_N^8-1+\sqrt{g_N^{16}-g_N^8+1}]=0\,.$$

c) Given that $G_{25}=(\sqrt{5}+1)/2$, show that

$$G_{225}=(2+\sqrt{3})^{1/3}\left(\frac{\sqrt{5}+1}{4}\right)[\sqrt{4+\sqrt{15}}+15^{1/4}]$$

and

$$G_{25/9}=(2+\sqrt{3})^{1/3}\left(\frac{\sqrt{5}+1}{4}\right)[\sqrt{4+\sqrt{15}}-15^{1/4}].$$

d) Given that $g_{58}^2 = (5+\sqrt{29})/2$, show that

$$g_{522} = \left(\frac{5+\sqrt{29}}{2}\right)^{1/2} (5\sqrt{29} + 11\sqrt{6})^{1/6} \left[\sqrt{\frac{9+3\sqrt{6}}{4}} + \sqrt{\frac{5+3\sqrt{6}}{4}}\right]$$

and

$$g_{58/9} = \left(\frac{5+\sqrt{29}}{2}\right)^{1/2} (5\sqrt{29} + 11\sqrt{6})^{1/6} \left[\sqrt{\frac{4+3\sqrt{6}}{4}} - \sqrt{\frac{9+3\sqrt{6}}{4}}\right].$$

14. a) Entry 23 in Chapter 18 of Ramanujan's second notebook (Berndt [Pr]) gives

i) $$\sqrt{2} \sum_{n=-\infty}^{\infty} \exp\left(\frac{-n^2\pi x}{x^2+y^2}\right) \cos\left(\frac{n^2\pi y}{x^2+y^2}\right)$$
$$= (\sqrt{x^2+y^2}+x)^{1/2} \sum_{n=-\infty}^{\infty} e^{-n^2\pi x} \cos(n^2\pi y)$$
$$+ (\sqrt{x^2+y^2}-x)^{1/2} \sum_{n=-\infty}^{\infty} e^{-n^2\pi x} \sin(n^2\pi y)$$

ii) $$\sqrt{2} \sum_{n=-\infty}^{\infty} \exp\left(\frac{-n^2\pi x}{x^2+y^2}\right) \sin\left(\frac{n^2\pi y}{x^2+y^2}\right)$$
$$= (\sqrt{x^2+y^2}-x)^{1/2} \sum_{n=-\infty}^{\infty} e^{-n^2\pi x} \cos(n^2\pi y)$$
$$- (\sqrt{x^2+y^2}+x)^{1/2} \sum_{n=-\infty}^{\infty} e^{-n^2\pi x} \sin(n^2\pi y).$$

Use Exercise 5 of Section 2.2 to prove these when x and y are complex with $\operatorname{re}(x \pm iy) > 0$.

b) Deduce that if $\operatorname{re}(s) > 0$,

$$\sum_{n=-\infty}^{\infty} e^{-n^2\pi s} \cos(n^2\pi s') = \frac{\sqrt{2}+\sqrt{1+s}}{\sqrt{1-s}} \sum_{n=-\infty}^{\infty} e^{-n^2\pi s} \sin(n^2\pi s').$$

c) Use ai) to deduce that

$$\theta_3(e^{-\pi}) = \sqrt{5\sqrt{5}-10}\,\theta_3(e^{-5\pi}).$$

d) Use b) with $s := \sqrt{5}/3$ to deduce that

$$(\sqrt{5}+3)\theta_3(e^{-\pi\sqrt{5}/3}) = (3+\sqrt{3})\theta_3(e^{-\pi 3\sqrt{5}}).$$

e) Use d) to conclude that

$$M(5) = \tfrac{1}{3}\sqrt{1+2\sqrt{3}+2\sqrt{5}}$$

and

$$G_{45}^{12} = \tfrac{1}{4}(\sqrt{5}+2)^3(\sqrt{5}+\sqrt{3})^4.$$

f) i) Use b) with $s := \sqrt{3}/2$ to obtain

$$k_{12} = (\sqrt{3}-\sqrt{2})^2(\sqrt{2}-1)^2 \quad \text{and} \quad g_{12}^{12} = \sqrt{2}(\sqrt{3}+1)^3.$$

ii) Use b) with $s := \sqrt{15}/4$ to obtain

$$\frac{k'_{15}}{k_{15}} = (4+\sqrt{15})(2+\sqrt{3})^2 \quad \text{and} \quad G_{15}^{12} = 4(7+3\sqrt{5}).$$

iii) Use b) with $s := \sqrt{7}/4$ to obtain

$$\frac{k'_7}{k_7} = 8+3\sqrt{7} \quad \text{and} \quad G_7^{12} = 8.$$

g) Use c) to show that

$$K(k_{25}) = \left(\frac{\sqrt{5}+2}{20}\right) \frac{\Gamma^2(\frac{1}{4})}{\sqrt{\pi}}.$$

15. a) As in Ewell [86] show that

$$\frac{\theta_4(q)^3}{\theta_4(q^3)} = 1 + 6\left\{\sum_{n=1}^{n=\infty} \frac{q^{3n-1}}{1+q^{3n-1}} - \frac{q^{3n-2}}{1+q^{3n-2}}\right\}$$

and so develop a formula for $r_3(n)$.
Hint: Use the quintuple-product of Section 9.4 and mimic the derivation of equation (9.1.14).

b) Evaluate

$$\sum_{n=1}^{n=\infty} 1/[1+F_{6n-3}].$$

Chapter Five

Modular Equations and Algebraic Approximations to π

Abstract. *In this chapter we study the algebraic relationships between elliptic integrals of the first and second kind. This study is applied to produce nth-order iteratons for π, rapid series for π^{-1}, and assorted other algebraic approximations to π.*

5.1 *SINGULAR VALUES OF THE SECOND KIND*

In Section 4.6 singular values were introduced. We will call λ^* the *singular value function* (*of the first kind*) where $\lambda^*(r) := k(e^{-\pi\sqrt{r}})$ as in Section 3.2. We introduce the *singular value function* (*of the second kind*) α which we define for positive r by

(5.1.1) $$\alpha(r) := \frac{E'}{K} - \frac{\pi}{4K^2} \qquad k := k(e^{-\pi\sqrt{r}}) = \lambda^*(r)\,.$$

Since $\lambda^*(r)$ tends to 0 as r tends to ∞, we have $\alpha(r)$ converging to π^{-1} as r increases. Indeed, as we shall see, the convergence is exponential which allows us to use $\alpha(r)$ to approximate $1/\pi$ effectively.

Using Legendre's identity and the fact that $K'(\lambda^*(r)) = \sqrt{r}K(\lambda^*(r))$, we have

(5.1.2) $$\alpha(r) = \frac{\pi}{4K^2} - \sqrt{r}\left(\frac{E}{K} - 1\right)$$

and $\qquad k := \lambda^*(r)$

(5.1.3) $$\alpha(r) = \sqrt{r}\,\frac{E'}{K'} - \frac{r\pi}{4K'^2}\,.$$

If in (5.1.2) we use the differential equation for K, equation (1.3.13), we may also write

(5.1.4) $$\alpha(r) = \frac{1}{\pi}\left(\frac{\pi}{2K}\right)^2 - \sqrt{r}\left(kk'^2\,\frac{\dot{K}}{K} - k^2\right) \qquad k := \lambda^*(r)\,.$$

Now since $\lambda^*(1/r) = \lambda^{*\prime}(r)$, we discover that

(5.1.5) $$\alpha(r^{-1}) = \frac{\sqrt{r} - \alpha(r)}{r}\,.$$

In particular $\alpha(1) = \frac{1}{2}$. We may rearrange (5.1.2) and (5.1.3) as follows:

(5.1.6) $$\frac{\pi}{4} = K[\sqrt{r}E - (\sqrt{r} - \alpha(r))K]$$

and $\qquad k := \lambda^*(r)$

(5.1.7) $$\frac{\pi}{4} = K'\left[\sqrt{r^{-1}}E' - \frac{\alpha(r)}{r}\,K'\right]$$

which may be viewed as one-sided forms of Legendre's identity. In the next sections we will give these identities substance by showing that $\alpha(r)$ is algebraic for rational r and by computing many values. Another useful equivalent form is

(5.1.8) $$E' = \sqrt{r}E - \delta(r)K$$

where $\qquad k := \lambda^*(r)$

(5.1.9) $$\delta(r) := \sqrt{r} - 2\alpha(r)\,.$$

Theorem 5.1

The function α is montonically decreasing for $r \geq 1$.

Proof. Since λ^* is decreasing, it suffices to show for $k < 1/\sqrt{2}$ that $f := (E'K - \pi/4)/K^2$ is an increasing function of k. This we establish by computing $\dot{f}$ and using the differential equations for E' and K. (See

Exercises 2 and 3 of Section 1.3.) We deduce from Legendre's identity that

$$\dot{f}(k) = \frac{\pi/2(E/K-1)+k^2E(K'-E')+(k')^2E'(K-E)}{k(k')^2K^2}$$

$$= \frac{k^2[(K-E)(E-\pi/(2K))+E(K'-E')-E(K-E)]+(k')^2(K-E)(E'-\pi/(2K))}{k(k')^2K^2}.$$

Since, for $k<1/\sqrt{2}$,

$$K \ge E \ge E' \ge 1 \ge \pi/2K$$

we finish by observing that, for $k<1/\sqrt{2}$,

$$K'-E' \ge K-E$$

and so substitution into the last equality completes the proof. □

We next provide a theta function expression for α. We combine (2.1.13) and (2.3.17) with (5.1.2) to write

$$\text{(5.1.10)} \qquad \alpha(r) = \frac{\pi^{-1}-\sqrt{r}4q\dot{\theta}_4/\theta_4}{\theta_3^4} \qquad \text{(w.r.t.}\,q)$$

where $q := e^{-\pi\sqrt{r}}$. Expanding this gives

$$\text{(5.1.11)} \qquad 0<\alpha(r)-\pi^{-1} = 8(\sqrt{r}-\pi^{-1})\,e^{-\pi\sqrt{r}}+O(re^{-2\pi\sqrt{r}})$$

$$\le 16\sqrt{r}e^{-\pi\sqrt{r}} \qquad r\ge 1$$

and

$$\text{(5.1.12)} \qquad 0<\alpha(r)-\pi^{-1} \le \sqrt{r}\lambda^{*2}(r).$$

One should compare (3.2.1).

Comments and Exercises

The function α is implicit in Ramanujan's work. In the next section we indicate how. Zucker [79] computes $\alpha(n)$ for $n := 1, 2, 3, 4, 5, 7$, while $\alpha(3)$ was known to Legendre. Formula (5.1.10) allows one to numerically compute α very easily.

1. a) Show that

$$\pi^{-1} = [\alpha(r)-\sqrt{r}\lambda^{*2}(r)]\theta_3^4(q)+4\sqrt{r}q\,\frac{\dot{\theta}_3(q)}{\theta_3(q)}$$

where $q := e^{-\pi\sqrt{r}}$.

b) Use a) to reprove Exercise 4b) of Section 2.3:

$$4\pi = \frac{\sum_{n=-\infty}^{\infty} e^{-n^2\pi}}{\sum_{n=-\infty}^{\infty} n^2e^{-n^2\pi}}.$$

2. By Exercise 4 of Section 1.6, $\lambda^*(2)=\sqrt{2}-1$. Use Theorem 1.2 to show that $\alpha(2)=\sqrt{2}-1$. Hence $\alpha(\frac{1}{2})=\frac{1}{2}$.

3. Prove (5.1.11) and (5.1.12).

5.2 CALCULATION OF α

We begin with an appropriate generalization of the quadratic transformation formula for E given in Theorem 1.2.

Propostion 5.1

Let $p>0$, $k := k(q)$, and $l := k(q^{1/p})$ be given. Then

$$\text{(5.2.1)} \quad pM_p^2(l,k)\left[\frac{E}{K}(k)-k'^2\right] = \frac{ll'^2}{M_p(l,k)}\,\frac{dM_p(l,k)}{dl}+\left[\frac{E}{K}(l)-l'^2\right].$$

Note: Herein $(dM_p(l,k)/dl)$ is the full derivative of $M_p(l,k)$ with respect to l.

Proof. We have $M_p(l,k)K(l)=K(k)$. We differentiate both sides with respect to k and use (4.6.2) to write

$$\text{(5.2.2)} \quad pM_p^2(l,k)\,\frac{kk'^2}{ll'^2}\,\frac{dK}{dk}(k) = M_p(l,k)\,\frac{dK}{dl}(l)+K(l)\,\frac{dM_p}{dl}(l,k).$$

Next we use the differential equation for K to write

$$\frac{dK}{dk}(k) = \frac{E(k)-k'^2K(k)}{kk'^2} \qquad \frac{dK}{dl}(l) = \frac{E(l)-l'^2K(l)}{ll'^2}$$

and we substitute these two identities into (5.2.2). We then have

$$pM_p^2(l,k)[E(k)-k'^2K(k)] = M_p(l,k)[E(l)-l'^2K(l)]+K(l)ll'^2\,\frac{dM_p(l,k)}{dl}.$$

On dividing each side by $K(k)$ we have (5.2.1). □

We now derive the key identity for α.

Theorem 5.2

For p and $r>0$ let $l:=\lambda^*(r)$ and $k:=\lambda^*(p^2r)$. Then

$$\alpha(p^2r)=M_p^{-2}(l,k)\alpha(r)-\sqrt{r}\left[M_p^{-2}(l,k)l^2-pk^2+\frac{pkk'^2}{M_p(l,k)}\frac{dM_p(l,k)}{dk}\right].$$
(5.2.3.)

Proof. We suppress variables in the multiplier when convenient. From (5.1.2) and (5.2.1) we have

$$\alpha(p^2r)=\frac{\pi}{4K^2(k)}-p\sqrt{r}\left[\frac{E}{K}(k)-1\right]$$
$$=M_p^{-2}\left\{\frac{\pi}{4K^2(l)}-\sqrt{r}\left[\frac{E}{K}(l)-1\right]-\sqrt{r}\left[l^2+\frac{ll'^2}{M_p}\frac{dM_p}{dl}-pM_p^2k^2\right]\right\}.$$

This gives

(5.2.4) $$\alpha(p^2r)=M_p^{-2}\left\{\alpha(r)-\sqrt{r}\left[l^2+\frac{ll'^2}{M_p}\frac{dM_p}{dl}-pM_p^2k^2\right]\right\}$$

on using (5.1.2) again. Another application of (4.6.2) produces the desired formula. □

In particular, if we let $r:=1/p$ above, then $l=k'$, and with (5.1.5) we derive that

(5.2.5) $$\alpha(p)=\sqrt{p}k^2-\frac{p}{2}k'k^2\frac{d}{dl}M_p(k',k)$$

or

(5.2.6) $$\alpha(p)=\sqrt{p}k^2-\frac{p}{2}kk'^2\frac{d}{dk}M_p(k',k)$$

where $k:=\lambda^*(p)$.

Let us observe that, since $\lambda^*(p)$ and M_p are algebraic for rational p, this shows that $\alpha(p)$ is algebraic for rational p.

EXAMPLE 5.1. When $p:=2$, $M_p(l,k)=1/(1+k)$ and $k=\lambda^*(2)=\sqrt{2}-1$. Then $dM_p(k',k)/dk=-\frac{1}{2}$ and $\alpha(2)=\sqrt{2}(\sqrt{2}-1)^2+(\sqrt{2}-1)^2=\sqrt{2}-1$. (Compare Exercise 2 of Section 1.) Similarly $\alpha(3)=(\sqrt{3}-1)/2$ and also $\alpha(7)=(\sqrt{7}-2)/2$. (See Exercise 3.)

Before continuing to evaluate α it is necessary to connect it to *Ramanujan's multiplier* (*of the second kind*).

(5.2.7) $$R_p(l,k):=\frac{pP(q)-P(q^{1/p})}{\theta_3^2(q)\theta_3^2(q^{1/p})}$$

where

(5.2.8) $$P(q):=1-24\sum_{n=1}^{\infty}\frac{nq^{2n}}{1-q^{2n}}.$$

Proposition 5.2

Let p, k, and l be as in Theorem 5.2. Then

$$R_p(l,k)=p(1-2k^2)M_p(l,k)-(1-2l^2)M_p^{-1}(l,k)+3pkk'^2\frac{dM_p(l,k)}{dk}.$$
(5.2.9)

Proof. We start with (3.2.15), which gives $\eta(q)/\eta(q^{1/p})$ in the form

$$\frac{q^{1/12}(1-q^2)(1-q^4)(1-q^6)\cdots}{q^{1/12p}(1-q^{2/p})(1-q^{4/p})(1-q^{6/p})\cdots}=\left(\frac{kk'}{ll'}\right)^{1/6}\sqrt{M_p(l,k)}.$$
(5.2.10)

We differentiate logarithmically and obtain

$$P(q)-\frac{1}{p}P(q^{1/p})=2q\frac{dk}{dq}\left[\frac{1}{kk'}\frac{d(kk')}{dk}-\frac{1}{ll'}\frac{d(ll')}{dl}\frac{dl}{dk}+\frac{3}{M_p}\frac{dM_p}{dk}\right].$$

Now we use (4.6.2) for dl/dk and (2.3.10) for qdk/dq and obtain

$$pP(q)-P(q^{1/p})=\frac{4LK}{\pi^2}\left[p(1-2k^2)M_p-(1-2l^2)M_p^{-1}+3pkk'^2\frac{dM_p}{dk}\right].$$

This gives (5.2.9). □

It is convenient to introduce two additional quantities:

(5.2.11) $$\varepsilon_p(l,k):=\frac{pkk'^2}{M_p(l,k)}\frac{dM_p(l,k)}{dk}+M_p^{-2}(l,k)l^2-pk^2$$

and

(5.2.12) $$\sigma(p):=R_p(k',k)\qquad k:=e^{-\pi\sqrt{p}}.$$

In these terms we have:

Theorem 5.3

(*a*) With r, p, k, and l as above, we have

$$\varepsilon_p(l, k) = \frac{M_p^{-1}(l, k)R_p(l, k) + (1 + l^2)M_p^{-2}(l, k) - p(1 + k^2)}{3} \tag{5.2.13}$$

$$\alpha(p^2 r) = M_p^{-2}(l, k)\alpha(r) - \sqrt{r}\varepsilon_p(l, k)\,. \tag{5.2.14}$$

(*b*) With $k = e^{-\pi\sqrt{p}} = \lambda^*(p)$, we have

$$\alpha(p) = \sqrt{p}\,\frac{1 + \lambda^*(p)^2}{3} - \frac{\sigma(p)}{6} \tag{5.2.15i}$$

$$\delta(p) = \frac{\sqrt{p}[1 - 2\lambda^*(p)^2] + \sigma(p)}{3}\,. \tag{5.2.15ii}$$

Proof. We deduce (5.2.13) and (5.2.14) by comparing (5.2.9) and (5.2.3). We obtain (5.2.15) on comparing (5.2.9) (with $l = k'$) to (5.2.6). □

Ramanujan has computed R_p for $p := 2, 3, 4, 5, 7, 11, 15, 17, 19, 23, 31, 35$. From these, many values of α are obtainable. The following table is taken from Ramanujan [14] with the entry for R_4 corrected.

The verification that R_p has the given form is tedious but straightforward for small p. [See Exercise 1c).] For larger p we rely on Ramanujan.

EXAMPLE 5.2. For $p := 7$, the modular equation in the form $(kl)^{1/4} + (k'l')^{1/4} = 1$ shows that $2k_7k_7' = \frac{1}{8}$ $k_7 := \lambda^*(7)$. Then $k_7 = (3 - \sqrt{7})/4\sqrt{2}$, and so $\sigma(7) = R_7(k_7', k_7) = 3(1 + 2k_7k_7') = 27/8$, $\alpha(7) = (\sqrt{7} - 2)/2$, and $\delta(7) = 2$.

We now make (5.2.14) explicit for $p := 2, 3, 4$.

Proposition 5.3

If $l := \lambda^*(r)$ and $k := \lambda^*(4r)$, then

$$(i)\quad k = \frac{1 - l'}{1 + l'}$$

and

$$(ii)\quad \alpha(4r) = (1 + k)^2\alpha(r) - 2\sqrt{r}k\,. \tag{5.2.16}$$

TABLE 5.1

p	$R_p(l, k)$
2	$l' + k$
3	$1 + kl + k'l'$
4	$\dfrac{3(1 + l')(1 + k)}{2}$
5	$(3 + kl + k'l')\sqrt{\dfrac{1 + kl + k'l'}{2}}$
7	$3(1 + kl + k'l')$
11	$2[2(1 + kl + k'l') + \sqrt{kl} + \sqrt{k'l'} - \sqrt{kk'll'}]$
15	$[1 + (kl)^{1/4} + (k'l')^{1/4}]^4 - (1 + kl + k'l')$
17	$[44(1 + k^2l^2 + k'^2l'^2) + 168(kl + k'l' - kk'll') - 102(1 - kl - k'l')(4kk'll')^{1/3} - 192(4kk'll')^{2/3}]^{1/2}$
19	$6[(1 + kl + k'l') + \sqrt{kl} + \sqrt{k'l'} - \sqrt{kk'll'}]$
23	$11(1 + kl + k'l') - 16(4kk'll')^{1/6}[1 + \sqrt{kl} + \sqrt{k'l'}] - 20(4kk'll')^{1/3}$
31	$3\{3(1 + kl + k'l') + 4(\sqrt{kl} + \sqrt{k'l'} + \sqrt{kk'll'}) - 4(kk'll')^{1/4}[1 + (kl)^{1/4} + (k'l')^{1/4}]\}$
35	$2[\sqrt{kl} + \sqrt{k'l'} - \sqrt{kk'll'}] + (4kk'll')^{-1/6}[1 - \sqrt{kl} - \sqrt{k'l'}]^3$

Proof. Since $R_2(l, k) = l' + k$ and $M_2^{-1}(l, k) = 2/(1 + l') = 1 + k$, we have

$$3\varepsilon_2(l, k) = (1 + k)^2(1 + l^2) - 2(1 + k^2) + (1 + k)(l' + k)$$

and

$$3\varepsilon_2(l, k) = \frac{4(1 + l^2) + 2(1 + l'^2) - 4(1 + l'^2)}{(1 + l')^2}$$

since $l' + k = (1 + l'^2)/(1 + l')$. Thus

$$\varepsilon_2(l, k) = \frac{2(1 - l'^2)}{(1 + l')^2} = 2k\,. \quad \square$$

For example,

$$\lambda^*(4) = (\sqrt{2} - 1)^2 \quad \text{and} \quad \alpha(4) = 2(\sqrt{2} - 1)^2\,.$$

Proposition 5.4

If $l := \lambda^*(r)$ and $k := \lambda^*(9r)$, then

$$(i)\quad M_3^{-1}(l, k) = \sqrt{1 + 4\frac{(kk')^{3/4}}{(ll')^{1/4}}} =: s(r)$$

and

$$(5.2.17)\qquad (ii)\quad \alpha(9r) = s^2(r)\alpha(r) - \frac{\sqrt{r}[s^2(r) + 2s(r) - 3]}{2}$$

where $m(r) := 3/s(r)$ satisfies

$$(iii)\quad m(9r) = \frac{([m^2(r) - 1]^{1/3} + 1)^2}{m(r)}.$$

Proof. (*i*) and (*iii*) were established in Section 4.7. For (*ii*) write

$$3\varepsilon_3(l, k) = s^2(r)(1 + l^2) + s(r)(1 + kl + k'l') - 3(1 + k^2).$$

Substitution in terms of α, as in Section 4.6, and some easy algebra yield $s(r) = 2\alpha + 1$ and

$$\varepsilon_3(l, k) = 2\alpha(\alpha + 2) = [s(r) - 1][s(r) + 3]/2$$

as claimed. □

A convenient variant of (5.2.17) is

$$(5.2.18)\qquad \delta(9r) = s^2(r)\delta(r) + 2\sqrt{r}s(r)$$

where, as before, $\delta(r) = \sqrt{r} - 2\alpha(r)$.

EXAMPLE 5.3. If $r := \frac{1}{3}$, then as in Section 4.6, $m(r) = s(r) = \sqrt{3}$. Then (5.2.17) gives $\alpha(3) = 3\alpha(\frac{1}{3}) - 1$. But (5.1.5) shows that $\alpha(3) = \sqrt{3} - 3\alpha(\frac{1}{3})$. Thus $\alpha(\frac{1}{3}) = (\sqrt{3} + 1)/6$ and $\alpha(3) = (\sqrt{3} - 1)/2$. Now we have $m(3) = (2^{1/3} + 1)^2/\sqrt{3}$ so that $s(3) = (4^{1/3} - 1)\sqrt{3}$ and $\delta(27) = 3(2^{4/3} - 1)$. Thus $\alpha(27) = 3[(\sqrt{3} + 1)/2 - 2^{1/3}]$.

Proposition 5.5

If $l := \lambda^*(r)$ and $k := \lambda^*(16r)$, then

$$(i)\quad \sqrt{k} = \frac{1 - \sqrt[4]{1 - l^2}}{1 + \sqrt[4]{1 - l^2}}$$

and

$$(5.2.19)\qquad (ii)\quad \alpha(16r) = (1 + y)^4\alpha(r) - 4\sqrt{r}y(1 + y + y^2)$$

where $y := \sqrt{k}$.

Proof. This may be derived similarly but is easily deduced from Proposition 5.2 and the quartic iteration of Exercise 3 of Section 1.4. □

EXAMPLE 5.4. For $r := 4$ we have $\alpha(4) = 2(\sqrt{2} - 1)$ and $\lambda^*(4) = (\sqrt{2} - 1)^2$. Thus $\sqrt{\lambda^*(64)} = (1 - 2^{5/8}\sqrt{\sqrt{2} - 1})/(1 + 2^{5/8}\sqrt{\sqrt{2} + 1}) = (\sqrt{\sqrt{2} + 1} - 2^{5/8})/(\sqrt{\sqrt{2} + 1} + 2^{5/8})$ and $\alpha(64) = 8[2(\sqrt{8} - 1) - (2^{1/4} - 1)^4]/(\sqrt{\sqrt{2} + 1} + 2^{5/8})^4$ which gives eight digits of π^{-1}. Similarly, $\sqrt{\lambda^*(16)} = (2^{1/4} - 1)/(2^{1/4} + 1)$ and $\alpha(16) = 4(\sqrt{8} - 1)/(2^{1/4} + 1)^4$.

Combining some of these calculations with (5.1.6) we have established that

$$\frac{\pi}{4} = K\left(\sqrt{3}E - \left(\frac{\sqrt{3} + 1}{2}\right)K\right)\qquad k := \frac{\sqrt{3} - 1}{2\sqrt{2}}$$

$$\frac{\pi}{4} = K\left(\sqrt{7}E - \left(\frac{\sqrt{7} + 2}{2}\right)K\right)\qquad k := \frac{3 - \sqrt{7}}{4\sqrt{2}}$$

and

$$\frac{\pi}{4} = K\left(3\sqrt{3}E - \left[3\left(\frac{\sqrt{3} - 1}{2} + 2^{1/3}\right)\right]K\right)\qquad k := \lambda^*(27)$$

with a similar identity whenever $\alpha(r)$ and $\lambda^*(r)$ are known.

Comments and Exercises

Computation of $\lambda^*(r)$ will be discussed further in Section 9.2. In many of the following numerical exercises the algebra is not entirely straightforward.

1. a) Verify that the quadratic case of (5.2.1) coincides with the formula given in Theorem 1.2.
b) Verify (5.2.6).
c) Verify that R_2, R_3, and R_4 are as claimed.

2. a) Show that in terms of Ramanujan's G_n and g_n of (3.2.13) one can write
i) $\lambda^*(n) = \frac{1}{2}G_n^{-3}[\sqrt{G_n^6 + G_n^{-6}} - \sqrt{G_n^6 - G_n^{-6}}]$
ii) $\lambda^*(n) = \frac{1}{2}[\sqrt{1 + G_n^{-12}} - \sqrt{1 - G_n^{-12}}]$
iii) $\lambda^*(n) = g_N^6[\sqrt{g_N^{12} + g_N^{-12}} - g_N^6]$.

b) Find similar identities for $\lambda^{*\prime}(n)$.
c) Verify the singular values given in (4.6.10).
d) In each following case, given G_n or g_n verify k_n. Then verify G_n or g_n.

i) $G_{15}^3 = 2^{-1/4}(\sqrt{5}+1)$,
$$k_{15} = (3-\sqrt{5})(\sqrt{5}-\sqrt{3})(2-\sqrt{3})/(8\sqrt{2})$$

ii) $G_{25}^3 = \sqrt{5}+2$, $k_{25} = (\sqrt{5}-2)(3-2\cdot 5^{1/4})/\sqrt{2}$

iii) $g_6^6 = \sqrt{2}+1$, $k_6 = (\sqrt{2}+1)(\sqrt{6}-\sqrt{2}-1)$
$$= (2-\sqrt{3})(\sqrt{3}-\sqrt{2})$$

iv) $g_{10}^6 = \sqrt{5}+2$, $k_{10} = (\sqrt{5}+2)(3\sqrt{2}-\sqrt{5}-2)$
$$= (\sqrt{10}-3)(\sqrt{2}-1)^2$$

v) $g_{18}^6 = 5+2\sqrt{6}$, $k_{18} = (5+2\sqrt{6})(7\sqrt{2}-5-2\sqrt{6})$.

3. Use (5.2.6) with $p := 3$ to compute $\alpha(3)$.

4. Use (5.2.15) to obtain the following values of α (or δ).

i) $\delta(5) = \sqrt{2(\sqrt{5}-1)}$

ii) $\delta(11) = [2x^2 - (x-\frac{3}{2}) - \sqrt{11}\sqrt{1-(x-\frac{3}{2})^2}]/3$

Note: $G_{11}^{-12} = x - \frac{3}{2}$ where $x^4 - x^3 = 2$.

iii) $\alpha(15) = (\sqrt{15}-\sqrt{5}-1)/2$.

5. Use (4.6.8) and (5.2.6) to compute $\delta(13) = (7+3\sqrt{13})G_{13}^{-6}$ where $G_{13}^{-4} = (\sqrt{13}-3)/2$.

6. Show that $R_p(l, k) = R_p(k', l')$, that $R_{p^{-1}}(k, l) = -p^{-1}R_p(l, k)$, and that $\sigma(p^{-1}) = -\sigma(p)/p$.

7. Use (5.2.14) to show that

i) $\delta(25) = 10\cdot 5^{1/4}(7-3\sqrt{5})$

ii) $2\lambda^*(49)\lambda^{*\prime}(49) = (1863+704\sqrt{7}) - (810+306\sqrt{7})\sqrt{2}\,7^{3/4}$
$$= \left(\frac{7^{1/4}-\sqrt{4+\sqrt{7}}}{2}\right)^{12}$$

and
$$\alpha(49) = \tfrac{7}{2} - \sqrt{7[\sqrt{2}\,7^{3/4}(33011+12477\sqrt{7}) - 21(9567+3616\sqrt{7})]}\,.$$

8. Use Proposition 5.3 to calculate

i) $\lambda^*(8) = (\sqrt{2}+1)^2(1-\sqrt{\sqrt{8}-2})^2$,
$\alpha(8) = (20+14\sqrt{2})(1-\sqrt{\sqrt{8}-2})^2$

ii) $\lambda^*(12) = (\sqrt{3}-\sqrt{2})^2(\sqrt{2}-1)^2$,
$\alpha(12) = 264+154\sqrt{3}-188\sqrt{2}-108\sqrt{6}$.

9. Use Proposition 5.4 to show that

i) $\alpha(18) = (21-6\sqrt{6})g_{18}^6\lambda^*(18)$

ii) $\delta(9) = 3^{3/4}(\sqrt{6}-\sqrt{2})$, as $m(1) = \sqrt{3+\sqrt{12}}$

iii) $\delta(81) = 9\sqrt{2}\,3^{1/4}(\sqrt{3}+1)(3+a)a^{-1}$, where $a := [(2+\sqrt{12})^{1/3}+1]^2$.

10. Prove Proposition 5.5.

11. a) Use (5.1.4) to write
$$\pi^{-1} = \sqrt{p}k'k^2\frac{\dot{\mathrm{AG}}(1,k')}{\mathrm{AG}(1,k')^3} + \frac{\alpha(p)-\sqrt{p}k^2}{\mathrm{AG}(1,k')^2}$$

where $k := \lambda^*(p)$ and the derivative is with respect to k.

b) Then (as in Section 2.5) show that
$$\pi = \lim_{i\to\infty}\frac{1}{\sqrt{p}k'k^2p_i + [\alpha(p)-\sqrt{p}k^2]q_i}$$

where $x_0 := 1/k'$, $q_1 := x_0$, $y_1 := \sqrt{x_0}$, and $p_1 := x_0^2/(x_0+1)$ while
$$x_{n+1} := \frac{\sqrt{x_n}+1/\sqrt{x_n}}{2}$$
$$y_{n+1} := \frac{y_n\sqrt{x_n}+1/\sqrt{x_n}}{y_n+1}$$
$$p_{n+1} := \left(\frac{1+y_n}{1+x_n}\right)p_n$$
$$q_{n+1} := \frac{q_n}{x_n}\,.$$

c) Show that convergence is quadratic.
d) When $p := 1$, this is Algorithm 2.1.

The next exercises develop results in J.M. Borwein [85] and Ramanujan [14]

12. a) Show that with P as in (5.2.8),
$$pP(e^{-\pi\sqrt{p}}) + P(e^{-\pi/\sqrt{p}}) = \frac{6\sqrt{p}}{\pi}\,.$$

Hint: Let $q := e^{-\pi\sqrt{p}}$ in (5.2.10) before differentiating.
Hence show that
$$P(e^{-\pi}) = \frac{3}{\pi}\,.$$

b) Show that

$$(5.2.20)\qquad P(e^{-\pi\sqrt{p}}) = \frac{\sigma(p)}{2\sqrt{p}}\,\mathrm{AG}^{-2}(1, \lambda^{*\prime}(p)) + \frac{3}{\pi\sqrt{p}}.$$

Thus $P(e^{-\pi\sqrt{p}})$ is quadratically computable.

c) Evaluate $P(e^{-\pi 3})$.

13. Show that

$$(5.2.21)\qquad \frac{3}{\pi} = 1 - \sum_{i=0}^{\infty} p^i\left[\frac{4K_iK_{i+1}}{\pi^2} R_p(k_i, k_{i+1}) - (p-1)\right]$$

where $K_i := K(k_i)$ and $k_i := \lambda^*(p^{2i})$. In J. M. Borwein [85] these identities are studied in detail.

14. Show that when $p := 2$, (5.2.21) is equivalent to Gauss's identity (2.5.9).

15. a) Show that

$$P(q) = \left[2\,\frac{K(k)}{\pi}\right]^2\left[3\,\frac{E}{K}\,(k) - (1 + k'^2)\right].$$

This identity, which follows from Exercise 7c) of Section 3.7, is entry 2 in Chapter 18 of Ramanujan's second notebook.

b) Prove that

$$P(q) = 1 - 24\sum_{n=1}^{\infty} \sigma_1(n) q^{2n}.$$

Here $\sigma_1(n)$ is the sum of the divisors of n, as in Exercise 12 of Section 3.7.

5.3 *FURTHER FORMULAE FOR* α

We commence by establishing a multiplication result for σ.

Theorem 5.4

Let $p, r > 0$ be given. Let $l := \lambda^*(1/pr)$, $\gamma := \lambda^*(p/r)$, and $k := \lambda^*(pr)$. Then

$$(5.3.1)\qquad \sigma(pr) = M_r^{-1}(\gamma, k)\left[R_p(l, \gamma) + \sqrt{\frac{p}{r}}\, R_r(\gamma, k)\right]$$

and

$$(5.3.2)\qquad \sigma\left(\frac{p}{r}\right) = M_r(\gamma, k)\left[R_p(l, \gamma) - \sqrt{\frac{p}{r}}\, R_r(\gamma, k)\right].$$

Proof. Let $s := pr$ and $q_1 = q^{1/r}$. Then $\gamma = k(q_1)$ and $l = k(q_1^{1/p})$. We have

$$R_s(l, k) = \frac{sP(q) - P(q^{1/s})}{\theta_3^2(q)\theta_3^2(q^{1/s})}$$

$$= \left[\frac{pP(q_1) - P(q_1^{1/p})}{\theta_3^2(q_1)\theta_3^2(q_1^{1/p})}\right]\frac{\theta_3^2(q^{1/r})}{\theta_3^2(q)} + p\left[\frac{rP(q) - P(q^{1/r})}{\theta_3^2(q)\theta_3^2(q^{1/r})}\right]\frac{\theta_3^2(q^{1/r})}{\theta_3^2(q^{1/s})}$$

so that with $\Gamma := K(\gamma)$,

$$(5.3.3)\qquad R_s(l, k) = R_p(l, \gamma)\,\frac{\Gamma}{K} + pR_r(\gamma, k)\,\frac{\Gamma}{L}.$$

For $k' = l$ we have $L = \sqrt{pr}K$ and (5.3.3) becomes

$$\sigma(pr) = \frac{\Gamma}{K}\left[R_p(l, \gamma) + \sqrt{\frac{p}{r}}\, R_r(\gamma, k)\right].$$

This is (5.3.1). Then (5.3.2) follows from (5.3.1) and Exercise 6 of Section 5.2. (See Exercise 1.) □

For $p = r$, (5.3.1) reduces to

$$(5.3.4)\qquad \sigma(p^2) = \frac{2R_p(1/\sqrt{2}, k)}{M_p(1/\sqrt{2}, k)}\qquad k := k(e^{-\pi p}).$$

Corollary 5.1

Let $p > 0$ and $k := \lambda^*(2p)$. Then

$$(5.3.5)\qquad \delta(2p) := \sqrt{\frac{p}{2}}\, k'^2 + \frac{1+k}{3}\, R_p\left(\frac{1-k}{1+k}, k\right).$$

Proof. Observe that $M_2^{-1}(\gamma, k) = 1 + k$ and $R_2(\gamma, k) = k + \gamma'$, while $\gamma' = (1-k)/(1+k)$. Then

$$\sigma(2p) = (1+k)\left[R_p(l, \gamma) + \sqrt{\frac{p}{2}}\,(k + \gamma')\right]$$

and since $R_p(l, \gamma) = R_p(\gamma', k)$,

$$(5.3.6)\qquad \sigma(2p) = (1+k)R_p\left(\frac{1-k}{1+k}, k\right) + \sqrt{\frac{p}{2}}\,(1 + k^2).$$

Now (5.3.5) follows from (5.2.15). □

EXAMPLE 5.5. For $p := 3$, $k = (2-\sqrt{3})(\sqrt{3}-\sqrt{2})$ while $R_3(\gamma, k) = 1 + \gamma k + \gamma' k'$. Now

$$(1+k)R_3\left(\frac{1-k}{1+k}, k\right) = 2k + k'^2 + 2\sqrt{k}k'$$

which we rewrite as $2k(1+\sqrt{2}g_6^6 + g_6^{12})$. Similarly $\sqrt{\tfrac{3}{2}}k'^2 = \sqrt{6}g_6^{12}k$, and we can write $\delta(6) = [\sqrt{6}(\sqrt{2}+1)^2 + 2\sqrt{2}(\sqrt{2}+1)]k$. Thus

$$\delta(6) = g_6^6\lambda^*(6)(2\sqrt{2}+2\sqrt{3}+\sqrt{6})$$

and

$$\alpha(6) = g_6^6\lambda^*(6)(3-\sqrt{2}) = 5\sqrt{6}+6\sqrt{3}-8\sqrt{2}-11. \quad \square$$

Corollary 5.2

Let $p>0$ and $l := \lambda^*(1/3p)$, $\gamma := \lambda^*(p/3)$, and $k := \lambda^*(3p)$. Then

$$\sigma(3p) = M_3^{-1}(\gamma, k)\left[R_p(\gamma', k) + \sqrt{\frac{p}{3}}\,(1+\gamma k+\gamma' k')\right] \tag{5.3.7}$$

and

$$\sigma\left(\frac{p}{3}\right) = M_3(\gamma, k)\left[R_p(\gamma', k) - \sqrt{\frac{p}{3}}\,(1+\gamma k+\gamma' k')\right] \tag{5.3.8}$$

where

$$M^{-1}\left(\frac{p}{3}\right) = M_3^{-1}(\gamma, k) = \sqrt{1+2\sqrt{2}\,\frac{G_{p/3}^3}{G_{3p}^9}}\,.$$

Proof. This follows from Theorem 5.4 and (4.7.9). (See Exercise 3.) $\square$

EXAMPLE 5.6. By piecing together various formulae many more values of α can be obtained. We illustrate this as follows. Given $\alpha(6)$ and $\lambda^*(6)$ from the previous example, we may use Proposition 5.3 to compute $\alpha(\tfrac{3}{2})$. Then the functional relation for α, equation (5.1.5), yields $\alpha(\tfrac{2}{3}) = (5\sqrt{6}-6\sqrt{3}-8\sqrt{2}+11)/3 = 0.5138118\ldots$. Similarly, given $\alpha(3)$ and $\lambda^*(3)$ from Example 5.3, we can use Proposition 5.3 to find that $\alpha(\tfrac{3}{4}) = 66+47\sqrt{2}-38\sqrt{3}-27\sqrt{6} = 0.5138837\ldots$.

Indeed numerical computation of the maximum of α [using (5.1.10) and Newton's method] shows that it occurs around 0.709 with a value of approximately 0.514275. [Note that $(\tfrac{2}{3}+\tfrac{3}{4})/2$ is very close to this point.] In addition, one may observe graphically that α increases up to this value and then decreases.

Comments and Exercises

From the given formulae and appropriate singular values, many values of α can be found in closed form. Some of the cleanest are given below.

1. Establish (5.3.2) of Theorem 5.4.

2. Use Corollary 5.1 and the given value of g_n to compute $\alpha(n)$ or $\delta(n)$.

i) $g_{10}^6 = \sqrt{5}+2$, $\quad\alpha(10) = g_{10}^6\lambda^*(10)(3\sqrt{5}-4)$

ii) $g_{18}^6 = (\sqrt{3}+\sqrt{2})^2$, $\quad\alpha(18) = g_{18}^6\lambda^*(18)(21-6\sqrt{6})$

iii) $g_{22}^2 = (\sqrt{2}+1)$, $\quad\alpha(22) = g_{22}^6\lambda^*(22)(33-17\sqrt{2})$

iv) $g_{58}^2 = (\sqrt{29}+5)/2$, $\quad\alpha(58) = g_{58}^6\lambda^*(58)(99\sqrt{29}-444)$.

(This requires having a tractable form of W_{29}, which we have not given but which may be found in Greenhill [1892].)

v) $\dfrac{g_{14}^6+g_{14}^{-6}}{2} = 2+\sqrt{2}$, $\quad\delta(14) = g_{14}^6\lambda^*(14)[(8+6\sqrt{2})+\sqrt{14}g_6^{14}]$

vi) $\dfrac{g_{30}^6+g_{30}^{-6}}{2} = 6+5\sqrt{2}$, $\quad\delta(30) = g_{30}^6\lambda^*(30)[(56+38\sqrt{2}) + \sqrt{30}g_{30}^6]$

vii) $\dfrac{g_{46}^6+g_{46}^{-6}}{2} = 18+13\sqrt{2}$, $\quad\delta(46) = g_{46}^6\lambda^*(46)[(200+142\sqrt{2}) + \sqrt{46}g_{46}^6]$.

3. Establish Corollary 5.2.

4. Use the values of G_{3p}, $G_{p/3}$, and $M(p/3)$ given in Exercises 8 and 9 of Section 4.7 to prove that:

i) $\sigma(21) = 3G_{21}^{-6}(11+6\sqrt{3}+2\sqrt{7}+\sqrt{21})$

ii) $\sigma\left(\dfrac{7}{3}\right) = G_{7/3}^{-6}(11-6\sqrt{3}+2\sqrt{7}-\sqrt{21})$

iii) $\sigma(33) = 3G_{33}^{-6}\sqrt{\dfrac{2\sqrt{3}+\sqrt{11}}{2}}\,(11+13\sqrt{3}+5\sqrt{11}+\sqrt{33})$

iv) $\sigma\left(\dfrac{11}{3}\right) = G_{11/3}^{-6}\sqrt{\dfrac{2\sqrt{3}-\sqrt{11}}{2}}\,(11+13\sqrt{3}-5\sqrt{11}-\sqrt{33})$

v) $\sigma(57) = 3G_{57}^{-6}\sqrt{\dfrac{2\sqrt{19}+5\sqrt{3}}{2}}\,(5\sqrt{57}+13\sqrt{19}+49\sqrt{3}+19)$

vi) $\sigma\left(\dfrac{19}{3}\right) = G_{19/3}^{-6}\sqrt{\dfrac{2\sqrt{19}-5\sqrt{3}}{2}}\,(5\sqrt{57}-13\sqrt{19}+49\sqrt{3}-19)$

and

vii) $\sigma(93) = 6G_{93}^{-6}\left(\frac{\sqrt{3}+1}{2}\right)^3(15\sqrt{93}+13\sqrt{31}+201\sqrt{3}+217)$

viii) $\sigma\left(\frac{31}{3}\right) = 2G_{31/3}^{-6}\left(\frac{\sqrt{3}-1}{2}\right)^3(15\sqrt{93}-13\sqrt{31}+201\sqrt{3}-217)$.

Hint: In each case express the right-hand-side of (5.3.7) or (5.3.8) as a function of $(\gamma\gamma' kk')^{1/4}$ by using the cubic modular equation (4.1.16).

5. The values of α given in Exercise 2 are all expressed in the form $\alpha(p) := g_p^6\lambda^*(p)a_p$ for a quadratic number a_p. This is also true for some other even p.

a) Since $g_p^6\lambda^*(p) \sim 1/(2g_p^6)$, deduce that

$$\pi_p := \frac{2g_p^6}{a_p} \sim \pi$$

and estimate the accuracy of the approximation.

b) Show that

$$\pi_{22} = \frac{14+10\sqrt{2}}{33-17\sqrt{2}} \quad \text{and} \quad \pi_{58} = \frac{140+26\sqrt{29}}{99\sqrt{29}-444}$$

which give four and eight digits of π, respectively.

6. a) Weber gives $G_{17}^2 + G_{17}^{-2} = (1+\sqrt{17})/2$ and $g_{34}^2 + g_{34}^{-2} = (3+\sqrt{17})/2$. Hence evaluate $\sigma(17)$ and $\sigma(34)$ as cleanly as possible.

b) Similarly, $f(\sqrt{-19}) =: x$ solves $x^3 = 2x+2$ and $f_1(\sqrt{-38}) =: \sqrt{2}x$ solves $x^3 = 2x^2 + (2x+1)(\sqrt{2}+1)$. Attempt to evaluate $\alpha(19)$ and $\alpha(38)$.

7. Use (5.3.4) to evaluate $\delta(25)$. (Compare Exercise 7 of Section 5.2.)

8. Given that $G_{37}^4 = \sqrt{37}+6$, one can show that

$$\delta(37) = (101 + 21\sqrt{37})G_{37}^{-6}.$$

Again we have not given a tractable form of W_{37}.

9. Show that the perimeter of an ellipse with major axis a and eccentricity k is given by

$$p = \frac{2a}{\sqrt{r}}\left[\frac{\pi}{2K(k)} + [\sqrt{r} + \delta(r)]K(k)\right]$$

where $k := \lambda^*(r)$. In particular, if $k := \tan(\pi/8)$,

$$p = a\sqrt{\frac{\pi}{4}}\left[\frac{\Gamma(\frac{1}{8})}{\Gamma(\frac{5}{8})} + \frac{\Gamma(\frac{5}{8})}{\Gamma(\frac{9}{8})}\right].$$

(See Exercise 4 of Section 1.6.) If $k := 1/\sqrt{2} = \sin(\pi/4)$

$$p = a\sqrt{\frac{\pi}{2}}\left[\frac{\Gamma(\frac{1}{4})}{\Gamma(\frac{3}{4})} + \frac{\Gamma(\frac{3}{4})}{\Gamma(\frac{5}{4})}\right].$$

Further such evaluations follow from Table 9.1, which gives $K(\lambda^*(n))$ in Γ terms for $1 \le n \le 16$.

5.4 RECURSIVE APPROXIMATION TO π

Theorem 5.3 is easily recast as a pth-order iterative method to compute π.

A General Iteration 5.1

Let p be a positive integer. Let $r > 0$ and set

$$\alpha_0 := \alpha(r) \quad \text{and} \quad k_0 := \lambda^*(r).$$

For n in $\mathbb{N}$ compute k_{n+1} by solving $W_p(k_n^2, k_{n+1}^2) = 0$ and let

(5.4.1)
$$m_n := M_p^{-1}(k_n, k_{n+1}) \qquad r_n := R_p(k_n, k_{n+1})$$
$$\varepsilon_n := [m_n r_n + m_n^2(1+k_n^2) - p(1+k_{n+1}^2)]/3$$

and

(5.4.2)
$$\alpha_{n+1} := m_n^2\alpha_n - p^n\sqrt{r}\varepsilon_n.$$

Then, for $rp^{2n} \ge 1$,

(5.4.3)
$$0 < \alpha_n - \pi^{-1} = 8(p^n\sqrt{r} - \pi^{-1})\, e^{-p^n\sqrt{r}\pi} + O(p^{2n}r\, e^{-p^n 2\sqrt{r}\pi})$$
$$\le 16p^n\sqrt{r}\, e^{-p^n\sqrt{r}\pi}.$$

Proof. This is a straightforward consequence of Theorem 5.3 and (5.1.11) because $\alpha_n := \alpha(p^{2n}r)$. □

We may also write this as an identity for π.

Theorem 5.5

Let p be a positive integer and let $r > 0$. Let m_n and ε_n be as in (5.4.1). Let $a_0 := 1$ and $a_{n+1} := m_n^{-1}a_n$. Then

(5.4.4)
$$\pi = \frac{AG^2(1, \lambda^{*\prime}(r))}{\alpha(r) - \sqrt{r}\,\Sigma_{n=0}^{\infty}\, p^n a_{n+1}^2 \varepsilon_n}.$$

Proof. Rewrite (5.4.2) as

$$a_{n+1}^2\alpha_{n+1} = a_n^2\alpha_n - \sqrt{r}p^n a_{n+1}^2\varepsilon_n . \tag{5.4.5}$$

Then summation yields

$$\alpha(r) - a_{m+1}^2\alpha_{m+1} = \sqrt{r}\sum_{n=0}^{m} p^n a_{n+1}^2\varepsilon_n$$

and, as α_m converges to π^{-1} while a_m converges to AG$(1, k_0')$ [since $a_m = K(k_m)/K(k_0)$], we obtain (5.4.4). □

EXAMPLE 5.7.

a) When $p := 2$, the proof of Proposition 5.3 shows that $\varepsilon_n = 2k_{n+1}$. In terms of the AGM: $a_{n+1}^2\varepsilon_n = 4a_{n+1}c_{n+1}/2 = c_n^2/2$, and (5.4.4) gives a family of identities extending (2.5.9), or Algorithm 2.2 (the case $r := 1$).
b) When $p := 3$, we similarly use Proposition 5.4 to deduce that $a_{n+1}^2\varepsilon_n = (a_n - a_{n+1})(a_n + 3a_{n+1})/2$, where $a_{n+1} = m_n^{-1}a_n$ can be computed from the cubic recursion in Proposition 5.4. (See also the cubic iteration given below.)

We now specialize Iteration 5.1, changing notation as appropriate.

A Quadratic Iteration 5.2

Let $r > 0$. Let $\alpha_0 := \alpha(r)$ and $k_0 := \lambda^*(r)$. For n in $\mathbb{N}$ let

$$k_{n+1} := \frac{1 - k_n'}{1 + k_n'} \tag{5.4.6i}$$

and

$$\alpha_{n+1} := (1 + k_{n+1})^2\alpha_n - 2^{n+1}\sqrt{r}k_{n+1} . \tag{5.4.6ii}$$

Then, for $r2^{2n} \geq 1$,

$$0 < \alpha_n - \pi^{-1} \leq 16 \cdot 2^n\sqrt{r}\, e^{-2^n\sqrt{r}\pi} .$$

A Quartic Iteration 5.3

Let $r > 0$. Let $\alpha_0 := \alpha(r)$ and $y_0 := \sqrt{\lambda^*(r)}$. For n in $\mathbb{N}$ let

$$y_{n+1} := \frac{1 - \sqrt[4]{1 - y_n^4}}{1 + \sqrt[4]{1 - y_n^4}} \tag{5.4.7i}$$

and

$$\alpha_{n+1} := (1 + y_{n+1})^4\alpha_n - 4^{n+1}\sqrt{r}y_{n+1}(1 + y_{n+1} + y_{n+1}^2) . \tag{5.4.7ii}$$

Then, for $r4^{2n} \geq 1$,

$$0 < \alpha_n - \pi^{-1} \leq 16 \cdot 4^n\sqrt{r}\, e^{-4^n\sqrt{r}\pi} .$$

Iteration 5.3 just peforms two steps of Iteration 5.2 as one, with some computational saving. The error bound given in each case is very accurate.

A Cubic Iteration 5.4

Let $r > 0$. Let $\alpha_0 := \alpha(r)$ and $m_0 := m(r) = \sqrt{1 + 2\sqrt{2}G_{9r}^3/G_r^9}$. For n in $\mathbb{N}$ let

$$m_{n+1} := \frac{[(m_n^2 - 1)^{1/3} + 1]^2}{m_n} \qquad s_n := \frac{3}{m_n} \tag{5.4.8i}$$

and

$$\alpha_{n+1} := s_n^2\alpha_n - 3^n\sqrt{r}\,\frac{s_n^2 + 2s_n - 3}{2} . \tag{5.4.8ii}$$

Then for $r3^{2n} \geq 1$,

$$0 < \alpha_n - \pi^{-1} \leq 16 \cdot 3^n\sqrt{r}\, e^{-3^n\sqrt{r}\pi} .$$

One can also provide a cubic iteration using k_n instead of s_n. This is somewhat more inelegant and no easier to initialize. [See Exercise 3b).]

Large numbers of initializations for Iterations 5.1, 5.2, and 5.3 are available in the previous sections. We collect some of the cleanest in Tables 5.2a) and b). The cubic information is given in Table 5.3. Recall that $[m(N) - 1][r(N) - 1] = 4$.

All the information necessary to verify these values lies in Section 4.7 and the previous sections of this chapter.

When $p := 7$ we can write the iteration cleanly in terms of $u_n := k_n^{1/4}$. Indeed

$$(1 - u_nu_{n+1})^8 = (1 - u_n^8)(1 - u_{n+1}^8) \tag{5.4.9}$$

while

$$m_n := \frac{7u_nu_{n+1}(1 - u_nu_{n+1})[1 - u_nu_{n+1} + (u_nu_{n+1})^2]}{u_n^8 - u_nu_{n+1}}$$

$$r_n := 3[1 + (u_nu_{n+1})^4 + (1 - u_nu_{n+1})^4]$$

and

$$\varepsilon_n := \frac{m_n^2(1 + u_n^8) + m_nr_n - 7(1 + u_{n+1}^8)}{3} .$$

TABLE 5.2a. Values of G_N^{-12} and $\alpha(N)$ for N odd

N	$2\lambda^*(N)\lambda^{*\prime}(N) = G_N^{-12}$	$\alpha(N)$
1	1	$\frac{1}{2}$
3	$\frac{1}{2}$	$\frac{\sqrt{3}-1}{2}$
5	$\sqrt{5}-2$	$\frac{\sqrt{5}-\sqrt{2\sqrt{5}-2}}{2}$
7	$\frac{1}{8}$	$\frac{\sqrt{7}-2}{2}$
9	$(2-\sqrt{3})^2$	$\frac{3-3^{3/4}\sqrt{2}(\sqrt{3}-1)}{2}$
13	$5\sqrt{13}-18$	$\frac{\sqrt{13}-\sqrt{74\sqrt{13}-258}}{2}$
15	$\frac{1}{8}\left(\frac{\sqrt{5}-1}{2}\right)^4$	$\frac{\sqrt{15}-\sqrt{5}-1}{2}$
25	$(\sqrt{5}-2)^4$	$\frac{5(1-2\cdot 5^{1/4}(7-3\sqrt{5}))}{2}$
27	$\frac{(2^{1/3}-1)^4}{2}$	$\frac{3(\sqrt{3}+1-2^{4/3})}{2}$
37	$(\sqrt{37}-6)^3$	$\frac{\sqrt{37}-(171-25\sqrt{37})(\sqrt{37}-6)^{1/2}}{2}$

TABLE 5.2b. Values of g_N^{-12} and $\alpha(N)$ for N even

N	$2\lambda^*(N)/\lambda^{*\prime 2}(N) = g_N^{-12}$	$\alpha(N)$
2	1	$\sqrt{2}-1$
4	$\frac{1}{2\sqrt{2}}$	$2(\sqrt{2}-1)^2$
6	$(\sqrt{2}-1)^2$	$(\sqrt{3}-\sqrt{2})(2-\sqrt{3})(3-\sqrt{2})(\sqrt{2}+1)$
10	$(\sqrt{5}-2)^2$	$(7+2\sqrt{5})(\sqrt{10}-3)(\sqrt{2}-1)^2$
18	$(\sqrt{3}-\sqrt{2})^4$	$3(\sqrt{3}+\sqrt{2})^4(\sqrt{6}-1)^2(7\sqrt{2}-5-2\sqrt{6})$
22	$(\sqrt{2}-1)^6$	$(\sqrt{2}+1)^6(33-17\sqrt{2})(3\sqrt{22}-7-5\sqrt{2})$
58	$\left(\frac{\sqrt{29}-5}{2}\right)^6$	$\left(\frac{\sqrt{29}+5}{2}\right)^6(99\sqrt{29}-444)(99\sqrt{2}-70-13\sqrt{29})$

TABLE 5.3. Selected cubic invariants

N	$m(N)$	$r(N)$	$\alpha(N)$
1/18	$3(3\sqrt{6}-4\sqrt{3}-5\sqrt{2}+7)$	—	$\frac{1019+416\sqrt{6}-720\sqrt{2}-588\sqrt{3}}{6}$
1/12	$6\sqrt{3}+9-4\sqrt{6}-6\sqrt{2}$	—	$\frac{47\sqrt{2}+27\sqrt{6}-38\sqrt{3}-66}{3}$
1/6	$(3-\sqrt{6})(\sqrt{2}+1)$	$(3+\sqrt{6})(\sqrt{2}+1)$	$\frac{8\sqrt{2}-4\sqrt{6}-6\sqrt{3}+11}{6}$
1/3	$\sqrt{3}$	$3+2\sqrt{3}$	$\frac{\sqrt{3}+1}{6}$
1/2	$\sqrt{6}-\sqrt{2}+1$	$\sqrt{6}+\sqrt{2}+1$	$\frac{1}{2}$
2/3	$\sqrt{3}(\sqrt{2}-1)(\sqrt{3}+\sqrt{2})$	$\sqrt{6}+\sqrt{3}$	$\frac{5\sqrt{6}-6\sqrt{3}-8\sqrt{2}+11}{3}$
1	$\sqrt{3+2\sqrt{3}}$	—	$\frac{1}{2}$
4/3	—	$\sqrt{3(2+\sqrt{3})}$	$\frac{2[54\sqrt{6}+77\sqrt{3}-94\sqrt{2}-132]}{3}$
2	$\sqrt{6}+\sqrt{2}-1$	$\sqrt{3}+\sqrt{2}$	$\sqrt{2}-1$
8/3	—	$\sqrt{3(\sqrt{3}+\sqrt{2})}$	$\frac{16(3\sqrt{6}+4\sqrt{2}-2)}{3[\sqrt{3}+1+\sqrt{2(\sqrt{3}-\sqrt{2})}]^4}$
3	$\frac{[1+2^{1/3}]^2}{\sqrt{3}}$	—	$\frac{\sqrt{3}-1}{2}$
4	—	$\sqrt{3+\sqrt{3}+\sqrt{9+6\sqrt{3}}}$	$6-4\sqrt{2}$
5	$\sqrt{1+2\sqrt{3}+2\sqrt{5}}$	—	$\frac{\sqrt{5}-\sqrt{2\sqrt{5}-2}}{2}$
6	—	$\frac{[\sqrt{2}(\sqrt{2}+1)^{2/3}+1]^2(\sqrt{2}-1)}{\sqrt{3}}$	$5\sqrt{6}+6\sqrt{3}-8\sqrt{2}-11$
7	$\left(\frac{6+\sqrt{21}+\sqrt{27+6\sqrt{21}}}{2}\right)^{1/2}$	—	$\frac{\sqrt{7}-2}{2}$
8	—	$\sqrt{(\sqrt{2}+1)(2+\sqrt{3})}$	$(2+\sqrt{2})^3(1-\sqrt{2\sqrt{2}-2})^2$
9	$\frac{[(2\sqrt{3}+2)^{1/3}+1]^2(\sqrt{3}-1)}{\sqrt{2}\cdot 3^{1/4}}$	—	$\frac{3-3^{3/4}\sqrt{2}(\sqrt{3}-1)}{2}$
18	—	$(\sqrt{3}-\sqrt{2})[1+(4+2\sqrt{6})^{1/3}]^2$	$3[721\sqrt{2}-1019+588\sqrt{3}-416\sqrt{6}]$

We present a few illustrations of the behaviour of the algorithms. We note that α_n in the quartic algorithm is just α_{2n} in the quadratic algorithm.

Digits Correct in Quadratic Algorithms

	$n=1$	2	3	4	5	6	7	8
$r=1$	0	3	8	19	41	84	171	344
$r=2$	2	5	13	28	56	120	242	489
$r=7$	5	12	26	55	112	227	458	919

Digits Correct in Cubic Algorithms

	$n=1$	2	3	4	5
$r=1$	2	10	34	107	327
$r=7$	8	30	93	288	873

Digits Correct in Septic Algorithms

	$n=1$	2	3
$r=1$	7	63	464
$r=7$	22	173	>1000

The updates for $\alpha(25r)$ and $\alpha(49r)$ are studied again in Section 9.5, where solvable versions of the quintic and septic iterations are given.

Comments and Exercises

Additional information on these iterations can be found in various of our papers. In particular, Borwein and Borwein [86] indicates the genesis of the quadratic iterations and [84*b*] that of the cubic iterations.

1. Verify the claims in Example 5.7.

2. a) Prove that, in the notation of Theorem 5.5,

$$\frac{E}{K}(k)=1-\sum_{n=0}^{\infty} p^n a_{n+1}^2 \varepsilon_n \qquad k=:k_0\,.$$

b) Observe that this extends Algorithm 1.2.

3. a) Verify Iterations 5.2, 5.3, and 5.4.
b) Use (4.1.24) to produce another form of the cubic iteration.

4. a) Determine the initial values for the cubic iteration with $r:=N/3$ and $N:=7,\ 11,\ 19,\ 31$.
b) Compute $\delta(45)$, $\delta(63)$, $\delta(243)$, and $\delta(54)$.

5. Derive the following version of the *septic* (seventh-order) *iteration*. Let $\alpha_0:=\alpha(r)$ and $u_0:=\lambda^*(r)^{1/4}$, and generate u_{n+1} decreasingly from

$$(1-u_n^8)(1-u_{n+1}^8)=(1-u_nu_{n+1})^8\,.$$

Let

$$a_n:=\frac{u_nu_{n+1}}{u_nu_{n+1}-u_{n+1}^8}$$

$$b_n:=\frac{7u_nu_{n+1}}{u_n^8-u_nu_{n+1}}$$

$$s_n:=\frac{b_n}{a_n}$$

$$t_n:=\frac{(1-u_{n+1}^8)(49a_n-b_n)+(1-u_n^8)(s_n-1)b_n}{8}$$

and

$$\alpha_{n+1}:=s_n\alpha_n+7^n\sqrt{r}(7-s_n-t_n)\,.$$

Then for $r7^{2n}\ge 1$,

$$0<\alpha_n-\pi^{-1}\le 16\cdot 7^n\sqrt{r}\,e^{-7^n\sqrt{r}\pi}\,.$$

6. Derive the following version of the *quintic* (fifth-order) *iteration* (given in Hughes [84]). Let $\alpha_0:=\alpha(r)$ and $u_0=\lambda^*(r)^{1/4}$, and generate u_{n+1} from $u_{n+1}^6-u_n^6-5(u_nu_{n+1})^2(u_n^2-u_{n+1}^2)-4u_nu_{n+1}[1-(u_nu_{n+1})^4]=0$. Let

$$x_n:=2u_nu_{n+1}^5$$

$$y_n:=2u_n^5u_{n+1}$$

$$a_n:=u_n^2+5u_{n+1}^2+2x_n$$

$$b_n:=5u_n^2+u_{n+1}^2-2y_n$$

$$c_n:=\frac{a_n}{b_n}$$

$$d_n:=\frac{(1-u_{n+1}^8)[5(u_{n+1}^2+x_n)+c_n(y_n-u_{n+1}^2)]}{4a_n}+\frac{(1-u_n^8)[u_n^2+x_n+5c_n(y_n-u_n^2)]}{4b_n}\,.$$

Then

$$\alpha_{n+1} := 5c_n\alpha_n + 5^{n+1}\sqrt{r}(d_n + u_{n+1}^8 - c_n u_n^8)$$

satisfies

$$0 < \alpha_n - \pi^{-1} \le 16 \cdot 5^n \sqrt{r}\, e^{-5^n\sqrt{r}\pi}$$

for $r5^{2n} \ge 1$.

7. Show that, in Iteration 5.1, convergence is indeed pth order.

Observe that for a variety of other values of p we have the information to make Iteration 5.1 entirely explicit. For example, $p := 17$ is satisfactory since we have R_{17}, and M_{17} is given in (4.6.9). Moreover, (4.6.9) also gives a form of the modular equation of order 17. Using $G_{17}^{12} + G_{17}^{-12} = 40 + 10\sqrt{17}$ and

$$\sigma^2(17) = \frac{(11\sqrt{17}+45)}{2}\left[(42+11\sqrt{17})\sqrt{\frac{13+5\sqrt{17}}{2}} - \frac{(397+77\sqrt{17})}{2}\right],$$

we have an algorithm for π which gives more than $\sqrt{17} \cdot 17^n$ digits at step n.

8. Let $p \ge 1$, let $l := \lambda^*(p)$ and $k := \lambda^*(49p)$. Set $z_p := (G_p G_{49p})^{-1}/\sqrt{2}$.

a) Show that

$$M_7(l,k) = \frac{2z_p(1-z_p)}{\sqrt{1-G_{49p}^{-24}} - \sqrt{1-4z_p}} = \frac{\sqrt{1-4z_p} - \sqrt{1-G_p^{-24}}}{14z_p(1-z_p)}.$$

b) Ramanujan [14] gives

$$G_{49}^{-1} = \frac{\sqrt{4+\sqrt{7}} - 7^{1/4}}{2}$$

and

$$G_{147}^{-1} = 2^{-1/12}\left\{\frac{1}{2} + \frac{1}{\sqrt{3}}\left[\frac{\sqrt{7}}{2} - (28)^{1/6}\right]\right\}.$$

Verify that

i) $M_7^{-1}\left(\frac{1}{\sqrt{2}}, \lambda^*(49)\right) = \dfrac{14z_1(1-z_1)}{\sqrt{1-4z_1}}$

where $z_1 = G_{49}^{-3}/\sqrt{2}$, and

ii) $M_7^{-1}(\lambda^*(3), \lambda^*(147)) = \dfrac{14z_3(1-z_3)}{\sqrt{1-4z_3} - \sqrt{3}/2}$

where

$$z_3 = \frac{[\sqrt{7}+\sqrt{3}-2(28)^{1/6}]^3}{48\sqrt{3}}.$$

c) Compute that

$$R_7(l,k) = 6(1-z_p)^2.$$

9. Verify, from Table 5.2, that

i) $\alpha(22) = (\sqrt{2}+1)^3(33-17\sqrt{2})(3\sqrt{11}-7\sqrt{2})(10-3\sqrt{11})$

and

ii) $\alpha(58) = (\sqrt{2}-1)^6(13\sqrt{58}-99)(99\sqrt{29}-444)\left(\dfrac{\sqrt{29}+5}{2}\right)^3.$

10. Ramanujan gives the following form of the modular equation of degree 7:

$$\left(\frac{x}{y}\right)^4 + \left(\frac{y}{x}\right)^4 + 7 = 2\sqrt{2}\{(xy)^3 + (xy)^{-3}\} \tag{5.4.10}$$

where $x := G_{49N}$ and $y := G_N$. This is Entry 19(ix) in Chapter 19 of the Second Notebook (Berndt [Pr]). One should compare Exercise 6 of Section 4.1 and Exercise 12 of Section 4.7.

a) Verify G_7, G_{49}, and G_{147}.

b) Show that

$$\left(\frac{x}{y}\right)^4 + \left(\frac{y}{x}\right)^4 - 7 = 2\sqrt{2}\{(xy)^3 + (xy)^{-3}\} \tag{5.4.11}$$

where $x := g_{49N}$ and $y := g_N$.

c) Verify that $g_{14}^2 + g_{14}^{-2} = \sqrt{2}+1$ and that

$$g_{98} + g_{98}^{-1} = \tfrac{1}{2}\{\sqrt{2} + \sqrt{14+4\sqrt{14}}\}.$$

5.5 *GENERALIZED ELLIPTIC INTEGRALS AND RATIONAL AND ALGEBRAIC SERIES FOR $1/\pi$ and $1/K$*

We begin with some results on hypergeometric functions [see (1.3.5)]. Changing notation slightly we write

(5.5.1) $${}_2F_1(a, b; c; x) := \sum_{n=0}^{\infty} \frac{(a)_n (b)_n}{(c)_n} \frac{x^n}{n!}$$

for appropriate values of the variables. Here we use the *rising factorial* or *Pochammer symbol* $(a)_n := \Gamma(a+n)/\Gamma(a) = a(a+1)(a+2)\cdots(a+n-1)$. Similarly the *generalized hypergeometric* function ${}_3F_2$ is defined by

(5.5.2) $${}_3F_2(a, b, c; d, e; x) := \sum_{n=0}^{\infty} \frac{(a)_n (b)_n (c)_n}{(d)_n (e)_n} \frac{x^n}{n!}$$

again where appropriate. (See Slater [66].) We define the *generalized complete elliptic integrals of the first and second kind* by

(5.5.3) $$K_s(k) := \frac{\pi}{2} \cdot {}_2F_1\left(\frac{1}{2} - s, \frac{1}{2} + s; 1; k^2\right)$$

and

(5.5.4) $$E_s(k) := \frac{\pi}{2} \cdot {}_2F_1\left(-\frac{1}{2} - s, \frac{1}{2} + s; 1; k^2\right)$$

for $|s| < \frac{1}{2}$ and $0 \le k \le 1$. We still denote the *complement* $k' := \sqrt{1-k^2}$ and write $K_s'(k) := K_s(k')$ and $E_s'(k) := E_s(k)$. Now $K := K_0$ and $E := E_0$ are the classical elliptic integrals, and each K_s and E_s admits many integral continuations. (See Erdélyi et al. [53, Section 2.12].) Moreover one has

(5.5.5) $$E_s = k'^2 K_s + \frac{kk'^2}{1+2s} \dot{K}_s .$$

This may be verified directly or by using Erdélyi et al. [53, Section 2.8]. [Here $\dot{K}_s = (d/dk)K_s$.] Similarly, using Erdélyi et al. [53, vol. 1(13), p. 85] we have

(5.5.6) $$E_s K_s' + K_s E_s' - K_s K_s' = \frac{\pi}{2} \frac{\cos(\pi s)}{1+2s} .$$

When $s = 0$, this is Legendre's relation (Section 1.6). The following relationships will be helpful.

Proposition 5.6

For $0 \le h \le 1/\sqrt{2}$ we have

(*a*) $\frac{2}{\pi} K_s(h) = {}_2F_1\left(\frac{1}{4} - \frac{s}{2}, \frac{1}{4} + \frac{s}{2}; 1; (2hh')^2\right)$

(*b*) $\left[\frac{2}{\pi} K_s(h)\right]^2 = {}_3F_2\left(\frac{1}{2} - s, \frac{1}{2} + s, \frac{1}{2}; 1, 1; (2hh')^2\right).$

Proof. (*a*) is a special case of Kummer's identity given in Rainville [60, p. 67] or in Erdélyi et al. [53, Section 2.11]. It may be verified by showing that both sides satisfy the appropriate hypergeometric differential equation (given in Exercise 7 of Section 1.3), are analytic, and agree at zero. (*b*) is a special case of Clausen's product for hypergeometric functions given in Slater [66, p. 75] and Exercise 13. □

In the sequel we will again use Ramanujan's invariants of (3.2.13)

(5.5.7) $$G := (2kk')^{-1/12} \qquad g := (2k/k'^2)^{-1/12}$$

and

$$2^{1/4} gG = (k^2/2k')^{-1/12} .$$

We also need Klein's *absolute invariant* J, which was introduced in Theorem 4.4. This is

(5.5.8) $$J := \frac{(4G^{24} - 1)^3}{27G^{24}} = \frac{(4g^{24} + 1)^3}{27g^{24}} .$$

Ramanujan [14] talks about "corresponding theories" for K_s, $s := \frac{1}{3}, \frac{1}{4}, \frac{1}{6}$, to that for K. For $s := \frac{1}{3}, \frac{1}{4}$ this is explained by the next result.

Proposition 5.7

(*a*) $K_{1/4}(h) = (1+k^2)^{1/2} K(k)$
if $2hh' = [(g^{12} + g)^{-12}/2]^{-1}$ and $0 \le h \le 1/\sqrt{2}$, $0 < k \le \sqrt{2} - 1$.

(*b*) $K_{1/3}(h) = [1 - (kk')^2]^{1/4} K(k)$
if $2hh' = J^{-1/2}$ and $0 \le h \le 1/\sqrt{2}$, $0 \le k \le 1/\sqrt{2}$.

Proof. These may be discovered by piecing together the quadratic and cubic transformations given in Erdélyi et al. [53, Section 2.11]. They may be verified by establishing that both sides satisfy the same differential equation (derived from the appropriate hypergeometric differential equation), and both functions involved have the same finite value at zero. □

There is a corresponding relation for $K_{1/6}$. Since it is a little less concise, we consider it at the end of the section. Combining these last two propositions leads to a variety of alternate hypergeometric expressions for K and K^2.

Theorem 5.6

(*a*) (*i*) $\frac{2K}{\pi}(k) = {}_2F_1\left(\frac{1}{4}, \frac{1}{4}; 1; (2kk')^2\right) \qquad 0 \le k \le \frac{1}{\sqrt{2}}$

(ii) $\dfrac{2K}{\pi}(k) = k'^{-1}{}_2F_1\left(\frac{1}{4}, \frac{1}{4}; 1; -\left(\frac{2k}{k'^2}\right)^2\right) \qquad 0 \le k \le \sqrt{2}-1$

(iii) $\dfrac{2K}{\pi}(k) = k'^{-1/2}{}_2F_1\left(\frac{1}{4}, \frac{1}{4}; 1; -\left(\frac{k^2}{2k'}\right)^2\right) \qquad 0 \le k^2 \le 2\sqrt{2}-2$

(b) (iv) $\dfrac{2K}{\pi}(k) = (1+k^2)^{-1/2}{}_2F_1\left(\frac{1}{8}, \frac{3}{8}; 1; \left(\frac{g^{12}+g^{-12}}{2}\right)^{-2}\right)$

$$0 \le k \le \sqrt{2}-1$$

(v) $\dfrac{2K}{\pi}(k) = (k'^2-k^2)^{-1/2}{}_2F_1\left(\frac{1}{8}, \frac{3}{8}; 1; -\left(\frac{G^{12}-G^{-12}}{2}\right)^{-2}\right)$

$$0 \le k \le \frac{2^{1/4}-\sqrt{2-\sqrt{2}}}{2}$$

(c) (vi) $\dfrac{2K}{\pi}(k) = [1-(kk')^2]^{-1/4}{}_2F_1\left(\frac{1}{12}, \frac{5}{12}; 1; J^{-1}\right) \qquad 0 \le k \le \frac{1}{\sqrt{2}}.$

Proof.

(a) We let $s := 0$ above to deduce (i). Then (ii) follows on replacing q by $-q$ in the theta function representations of K and $(2kk')^2$. This is Jacobi's imaginary transformation of Exercise 7d) in Section 3.2. We derive (iii) from (ii) by replacing k by $k_1 := (1-k')/(1+k')$ and using the quadratic transformation $K(k_1) = [(1+k')/2]K(k)$ of Theorem 1.2.

(b) (iv) comes from letting $s := \frac{1}{4}$ above. Then (v) again follows from Jacobi's imaginary transformation.

(c) (vi) comes from letting $s := \frac{1}{3}$ above. □

Similarly,

Theorem 5.7

For k restricted as in Theorem 5.6

(a) (i) $\left[\dfrac{2K}{\pi}(k)\right]^2 = {}_3F_2\left(\frac{1}{2}, \frac{1}{2}, \frac{1}{2}; 1, 1; (2kk')^2\right)$

(ii) $\left[\dfrac{2K}{\pi}(k)\right]^2 = k'^{-2}{}_3F_2\left(\frac{1}{2}, \frac{1}{2}, \frac{1}{2}; 1, 1; -\left(\frac{2k}{k'^2}\right)^2\right)$

(iii) $\left[\dfrac{2K}{\pi}(k)\right]^2 = k'^{-1}{}_3F_2\left(\frac{1}{2}, \frac{1}{2}, \frac{1}{2}; 1, 1; -\left(\frac{k^2}{2k'}\right)^2\right)$

(b) (iv) $\left[\dfrac{2K}{\pi}(k)\right]^2 = (1+k^2)^{-1}{}_3F_2\left(\frac{1}{4}, \frac{3}{4}, \frac{1}{2}; 1, 1; \left(\frac{g^{12}+g^{-12}}{2}\right)^{-2}\right)$

(v) $\left[\dfrac{2K}{\pi}(k)\right]^2 = (k'^2-k^2)^{-1}{}_3F_2\left(\frac{1}{4}, \frac{3}{4}, \frac{1}{2}; 1, 1; -\left(\frac{G^{12}-G^{-12}}{2}\right)^{-2}\right)$

(c) (vi) $\left[\dfrac{2K}{\pi}(k)\right]^2 = [1-(kk')^2]^{-1/2}{}_3F_2\left(\frac{1}{6}, \frac{5}{6}, \frac{1}{2}; 1, 1; J^{-1}\right).$

Proof. We combine Theorem 5.6 and Proposition 5.6. □

Thus we have provided series for K and K^2 in terms of each of the six invariants. One can produce other such formulae by further use of transformation identities. For example, Bailey's formula in Erdélyi et al. [53, (2), Section 4.5] with $a := \frac{1}{2}$ and $b := 1$ gives

$$\left[\frac{2K}{\pi}(k)\right]^2 = [1-4(2kk')^2]^{-1/2}{}_3F_2\left(\frac{1}{6}, \frac{5}{6}, \frac{1}{2}; 1, 1; \frac{-27(2kk')^2}{[1-4(2kk')^2]^3}\right)$$

(5.5.9) $$= (k'^4+16k^2)^{-1/2}{}_3F_2\left(\frac{1}{6}, \frac{5}{6}, \frac{1}{2}; 1, 1; \frac{27g^{48}}{(g^{24}+4)^3}\right).$$

Note also that we may use (5.5.5) with $s := 0$ and Theorem 5.6 to produce similar series for E. We are now ready to build our series. Recall (5.1.4), which we write as

$$\frac{1}{\pi} = \sqrt{N}k_N k_N'^2 \frac{4K\dot{K}}{\pi^2} + [\alpha(N) - \sqrt{N}k_N^2]\frac{4K^2}{\pi^2} \qquad k_N := \lambda^*(N)$$

(5.5.10)

or

$$\frac{1}{K} = \sqrt{N}k_N k_N'^2 \frac{4\dot{K}}{\pi} + [\alpha(N) - \sqrt{N}k_N^2]\frac{4K}{\pi} \qquad k_N := \lambda^*(N).$$

(5.5.11)

Thus given $\alpha(N)$ and $\lambda^*(N)$, we can combine (5.5.10) with Theorem 5.7 to produce series for $1/\pi$. In like fashion we derive series for $1/K$ or for the Gaussian AGM, $M(1,k') = \pi/2K$. In each case we have $[(2K/\pi)(k)]^2 = m(k)F(\phi(k))$ for algebraic m and ϕ, while $F(\phi)$ has a hypergeometric-type power series expansion $\Sigma_{n=0}^{\infty} a_n\phi^n$. Then $4K\dot{K}/\pi^2 = \frac{1}{2}\dot{m}F + \frac{1}{2}m\dot{\phi}\dot{F}(\phi)$. Substitution in (5.5.10) leads to

$$\frac{1}{\pi} = \sum_{n=0}^{\infty} a_n\left[\frac{\sqrt{N}}{2}kk'^2\dot{m} + [\alpha(N) - \sqrt{N}k^2]m + \frac{n\sqrt{N}}{2}m\frac{\dot{\phi}}{\phi}kk'^2\right]\phi^n.$$

(5.5.12)

Thus for rational N, the bracketed term is of the form $a + nb$ with a and b algebraic. We now specialize this for our invariants.

SERIES IN G_N: For $N > 1$,

(5.5.13) $$\frac{1}{\pi} = \sum_{n=0}^{\infty} \left[\frac{(\frac{1}{2})_n}{n!}\right]^3 a_n(N)(G_N^{-12})^{2n}$$

where

$$a_n(N) := [\alpha(N) - \sqrt{N}k_N^2] + n\sqrt{N}(k_N'^2 - k_N^2).$$

SERIES IN g_N: For $N \geq 2$,

(5.5.14) $$\frac{1}{\pi} = \sum_{n=0}^{\infty} (-1)^n \left[\frac{(\frac{1}{2})_n}{n!}\right]^3 b_n(N)(g_N^{-12})^{2n}$$

where

$$b_n(N) := \alpha(N)k_N'^{-2} + n\sqrt{N}\left(\frac{1+k_N^2}{1-k_N^2}\right).$$

SERIES IN $g_{4N} = 2^{1/4}g_N G_N$: For $N \geq \frac{1}{2}$,

(5.5.15) $$\frac{1}{\pi} = \sum_{n=0}^{\infty} (-1)^n \left[\frac{(\frac{1}{2})_n}{n!}\right]^3 c_n(N)(g_{4N}^{-12})^{2n}$$

where

$$c_n(N) := \left[\alpha(N) - \frac{\sqrt{N}}{2} k_N^2\right]k_N'^{-1} + n\sqrt{N}(k_N' + k_N'^{-1}).$$

SERIES IN $x_N := \left(\dfrac{g_N^{12} + g_N^{12}}{2}\right)^{-1} = \dfrac{4k_N k_N'^2}{(1+k_N^2)^2}$. For $N > 2$,

(5.5.16) $$\frac{1}{\pi} = \sum_{n=0}^{\infty} \frac{(\frac{1}{4})_n(\frac{1}{2})_n(\frac{3}{4})_n}{(n!)^3} d_n(N)x_N^{2n+1}$$

where

$$d_n(N) := \left[\frac{\alpha(N)x_N^{-1}}{1+k_N^2} - \frac{\sqrt{N}}{4} g_N^{-12}\right] + n\sqrt{N}\left(\frac{g_N^{12} - g_N^{-12}}{2}\right).$$

SERIES IN $y_N := \left(\dfrac{G_N^{12} - G_N^{-12}}{2}\right)^{-1} = \dfrac{4k_N k_N'}{1 - 4(k_N k_N')^2}$. For $N \geq 4$,

(5.5.17) $$\frac{1}{\pi} = \sum_{n=0}^{\infty} (-1)^n \frac{(\frac{1}{4})_n(\frac{1}{2})_n(\frac{3}{4})_n}{(n!)^3} e_n(N)y_N^{2n+1}$$

where

$$e_n(N) := \left[\frac{\alpha(N)y_N^{-1}}{k_N'^2 - k_N^2} + \frac{\sqrt{N}}{2} k_N^2 G_N^{12}\right] + n\sqrt{N}\left(\frac{G_N^{12} + G_N^{-12}}{2}\right).$$

SERIES IN J_N^{-1}. For $N > 1$,

(5.5.18) $$\frac{1}{\pi} = \sum_{n=0}^{\infty} \frac{(\frac{1}{6})_n(\frac{1}{2})_n(\frac{5}{6})_n}{(n!)^3} f_n(N)(J_N^{-1/2})^{2n+1}$$

where

$$f_n(N) := \frac{1}{3\sqrt{3}}[\sqrt{N}\sqrt{1 - G_N^{-24}} + 2(\alpha(N) - \sqrt{N}k_N^2)(4G_N^{24} - 1)]$$
$$+ n\sqrt{N}\frac{2}{3\sqrt{3}}[(8G_N^{24} + 1)\sqrt{1 - G_N^{-24}}].$$

There are many rearrangements of these formulae. In similar fashion we may deduce that for all N,

(5.5.19) $$M(1, k_N') = \frac{\pi}{2K(k_N)} = \pi \sum_{n=0}^{\infty} m_n(N)\left[\frac{(\frac{1}{2})_n}{n!}\right]^2 k_N^{2n}$$

where

$$m_n(N) := [\alpha(N) - \sqrt{N}k_N^2] + n2\sqrt{N}k_N'^2$$

and for $N > 1$,

(5.5.20) $$M(1, k_N') = \pi \sum_{n=0}^{\infty} (-1)^n n_n(N)\left[\frac{(\frac{1}{2})_n}{n!}\right]^2 \left(\frac{k_N}{k_N'}\right)^{2n}$$

where

$$n_n(N) := \alpha(N)k_N'^{-1} + n2\sqrt{N}k_N'^{-1}.$$

These use the hypergeometric definition of K and (5.5.11). Also using (5.5.11) and Theorem 5.6(*ai*) and (*aii*) leads to, for $N > 1$, (5.5.21) $$M(1, k'_N) = \pi \sum_{n=0}^{\infty} o_n(N)\left[\frac{(\frac{1}{4})_n}{n!}\right]^2 (G_N^{-12})^{2n}$$

where

$$o_n(N) := [\alpha(N) - \sqrt{N}k_N^2] + n2\sqrt{N}(k_N'^2 - k_N^2)$$

and for $N \geq 2$,

(5.5.22) $$M(1, k'_N) = \pi \sum_{n=0}^{\infty} (-1)^n p_n(N)\left[\frac{(\frac{1}{4})_n}{n!}\right]^2 (g_N^{-12})^{2n}$$

where

$$p_n(N) = \alpha(N)k_N'^{-1} + n2\sqrt{N}[1 + k_N^2]k_N'^{-1}.$$

Similar formulae exist in the other invariants.

From our formulae for π^{-1} and the values of $\alpha(N)$ and $\lambda^*(N) = k_N$ previously derived we have explicitly computed all but two of the 14 series which Ramanujan gives without justification in [14, Section 14]. Ramanujan gives series of the form (5.5.13) for $N := 3, 7, 15$, of the form (5.5.16) for $N := 6, 10, 18, 22, 58$, and of the form (5.5.17) for $N := 5, 9, 13, 25, 37$. He gives series of the form (5.5.18) for $N := 3$ and 7 and two in terms of $K_{1/6}$ which we derive below. In each case manipulation of the formulae produces the desired result. Indeed $\alpha(37)$ and $\alpha(58)$ were obtained by calculating $e_0(37)$ and $d_0(58)$ to high precision. In fact, with $N := 58$, using (5.5.16) and Exercise 2 of Section 5.3 produces

(5.5.23) $$\frac{1}{\pi} = 2\sqrt{2} \sum_{n=0}^{\infty} \frac{(\frac{1}{4})_n(\frac{1}{2})_n(\frac{3}{4})_n}{(n!)^3} (1103 + 26390n)\left(\frac{1}{99^2}\right)^{2n+1}$$

which adds eight digits a term! Since k_N^2 behaves like $16e^{-\pi\sqrt{N}}$, it is very easy to estimate the convergence rate in each series. For N at all large, the rate while linear is most impressive. In the exercises we give various other examples. Bailey [35, p. 96] gives (5.5.14) with $N := 2$ [equivalently (5.5.15) with $N := \frac{1}{2}$] and ascribes this to Ramanujan. The series is

(5.5.24) $$\frac{2}{\pi} = \sum_{n=0}^{\infty} (-1)^n \left[\frac{(\frac{1}{2})_n}{n!}\right]^3 (4n+1).$$

Correspondingly, (5.5.22) with $N := 2$ yields

(5.5.25) $$M(1, 1/k'_2) = \frac{\pi}{2} \sum_{n=0}^{\infty} (-1)^n \left[\frac{(\frac{1}{4})_n}{n!}\right]^2 (8n+1),$$

while for $N := 1$, the series in (5.5.20) diverges.

We now return to $K_{1/6}$. From Goursat's exhaustive list of transformations (Goursat [1881]) we obtain:

Proposition 5.8

For $k < 1/\sqrt{2}$ and h the smaller of the two real solutions of

(5.5.26) $$\frac{(9-8h^2)^3}{64h^6h'^2} = J(k) = \frac{(4G^{24}-1)^3}{27G^{24}}$$

one has

(5.5.27) $$\left(\frac{2K}{\pi}\right)^2(k) = \sqrt{\frac{1-\frac{8}{9}h^2}{1-(kk')^2}}\left(\frac{2K_{1/6}}{\pi}\right)^2(h).$$

Proof. Formula (126) in Goursat [1881] and Propositions 5.6 and 5.7 combine to produce (5.5.26) and (5.5.27). □

There is a corresponding formula for the larger solution. This implicit formula for l in terms of k can be solved explicitly as follows (Exercise 19). For $h \leq (\sqrt{3}+1)/2\sqrt{2}$,

(5.5.28*i*) $$H^{24} := (2hh')^{-2} = \left(\frac{\sqrt{x} + 1/\sqrt{x}}{2}\right)^2$$

where

(5.5.28*ii*) $$x := \left(\frac{2\Delta - 3}{9}\right) + \frac{2}{9}\sqrt{3 + 2(J^{1/3}-1)\Delta - \Delta^2}$$

and

(5.5.28*iii*) $$\Delta := \sqrt{1 + J^{1/3} + J^{2/3}}.$$

In each case ($s := \frac{1}{3}, \frac{1}{4}, \frac{1}{6}$) the transformation from k to h can be described very simply analytically. Consider the generalized singular value function λ_s^* defined by

(5.5.29) $$\frac{K_s'(\lambda_s^*(N))}{K_s(\lambda_s^*(N))} = \sqrt{N} \qquad N > 0.$$

Then it transpires that in all three cases,

(5.5.30) $$\sqrt{C_s}\,\frac{K_s'(\lambda_s^*(N))}{K_s(\lambda_s^*(N))} = \frac{K'(\lambda^*(C_sN))}{K(\lambda^*(C_sN))} \qquad C_s := 4\cos^2(\pi s).$$

(This can be verified from formulae in Goursat [1881].) In other words, the Nth singular value of K is sent to the Nth, $(N/2)$th and $(N/3)$th singular values of $K_{1/3}$, $K_{1/4}$, and $K_{1/6}$, respectively. Thus

$$\text{(5.5.31}i\text{)} \qquad \left(\frac{g_{2N}^{12}+g_{2N}^{-12}}{2}\right)^{-1} = 2\lambda_{1/4}^*(N)\lambda_{1/4}^{*\prime}(N)$$

and

$$\text{(5.5.31}ii\text{)} \qquad J_N^{-1/2} = 2\lambda_{1/3}^*(N)\lambda_{1/3}^{*\prime}(N)\,,$$

while various singular values for $K_{1/6}$ are given in Exercise 19b). If we now define α_s by

$$\text{(5.5.32)} \qquad \alpha_s(N) = \frac{\pi}{4K_s^2}\,\frac{\cos(\pi s)}{1+2s} - \sqrt{r}\left(\frac{E_s}{K_s}-1\right) \qquad k := \lambda_s^*(N)$$

we may use (5.5.5) and (5.5.6) to write

$$\text{(5.5.33)} \qquad \frac{1}{\pi} = \sum_{n=0}^{\infty}[a_s(N)+nb_s(N)]\left[\frac{(\frac{1}{2}-s)_n(\frac{1}{2}+s)_n(\frac{1}{2})_n}{(n!)^3}\right]G_s^{-24n}(N)$$

where

$$\text{(5.5.34}i\text{)} \qquad a_s(N) := [\alpha_s(N) - \sqrt{N}\lambda_s^{*2}(N)]\,\frac{1+2s}{\cos(\pi s)}$$

$$\text{(5.5.34}ii\text{)} \qquad b_s(N) := \sqrt{N}\sqrt{1-G_s^{-24}(N)}\,\frac{1}{\cos(\pi s)}$$

while

$$G_s^{-12}(N) := 2\lambda_s^*(N)\lambda_s^{*\prime}(N)\,.$$

The details are left as Exercise 20. Now, with some perseverance, we can derive series including Ramanujan's missing formulae, which come with $s := \frac{1}{6}$ and $N := 4$ and 5 in (5.5.33) [See Exercise 20b).]

Finally, we observe that the result of Exercise 22 in combination with the discussion of Γ values in Section 9.2 shows that the formulae for $K_{1/3}$, $K_{1/4}$, and $K_{1/6}$ are in essence the only such formulae.

Comments and Exercises

In Section 13 of Ramanujan [14] one finds an explanation of series of the form (5.5.13) without many details. Then in Section 14, with essentially no explanation, he gives his other 14 series. Hardy quoting Mordell (in Ramanujan [62]) observes that "it is unfortunate that Ramanujan has not developed in detail the corresponding theories." The explanation as provided by this section is a bit disappointing, since for all these theories, all we have are well-concealed versions of the original theory for K. Nonetheless we can explain all of the beautiful and mysterious series.

1. Prove the generalized Legendre identity of (5.5.6).

2. Prove Proposition 5.7.

3. Verify formulae (5.5.13) to (5.5.23).

4. Show that

$$\frac{4}{\pi} = \sum_{n=0}^{\infty}(-1)^n\frac{(\frac{1}{4})_n(\frac{1}{2})_n(\frac{3}{4})_n}{(n!)^3}(1123+21460n)\left(\frac{1}{882}\right)^{2n+1}.$$

5. Show that

$$\frac{\sqrt{2}}{\pi 3^{1/4}} = \sum_{n=0}^{\infty}\left[\frac{(\frac{1}{2})_n}{n!}\right]^3[(3-\sqrt{3})+12n](2-\sqrt{3})^{4n+1}.$$

6. Show that

$$\frac{2}{3\pi} = \sum_{n=0}^{\infty}(-1)^n\left[\frac{(\frac{1}{2})_n}{n!}\right]^3[(7-2\sqrt{6})+28n](\sqrt{3}-\sqrt{2})^{8n+2}.$$

7. Show that in (5.5.18)

$$f_n(2) = (28n+3)\sqrt{3}/9 \qquad J_2^{-1} = (\tfrac{3}{5})^3$$

while

$$f_n(4) = (63n+5)\sqrt{6}/3 \qquad J_4^{-1} = (\tfrac{2}{11})^3$$

and

$$f_n(7) = (133n+8)9\sqrt{3}/4 \quad J_7^{-1} = (\tfrac{4}{85})^3\,.$$

8. Show that

$$M\left(1,\frac{1}{\sqrt{2}}\right) = \pi\sum_{n=0}^{\infty}n\left[\frac{(\frac{1}{2})_n}{n!}\right]^2 2^{-n}.$$

9. Show that

$$M\left(1,\frac{\sqrt{3}+1}{2\sqrt{2}}\right) = \frac{\pi}{4}\sum_{n=0}^{\infty}(12n+1)\left[\frac{(\frac{1}{4})_n}{n!}\right]^2 4^{-n}$$

and

$$M\left(1, \frac{\sqrt{7}+3}{4\sqrt{2}}\right) = \frac{\pi}{16}\sum_{n=0}^{\infty}(84n+5)\left[\frac{(\frac{1}{4})_n}{n!}\right]^2 64^{-n}.$$

10. Show that

$$2\sqrt{2}M(2^{1/4}, 2^{-1/4}) = \pi\sum_{n=0}^{\infty}(-1)^n(12n+1)\left[\frac{(\frac{1}{4})_n}{n!}\right]^2 8^{-n}.$$

11. a) Show, using (5.5.13) with $n := 7$, that

$$\frac{1}{\pi} = \sum_{n=0}^{\infty}\binom{2n}{n}^3\frac{42n+5}{2^{12n+4}}.$$

This series of Ramanujan's has the property that, as J. Holloway has observed, it can be used to compute the millionth (binary) digit of $1/\pi$ without computing the first half million digits. Note that the terms are exact binary fractions whose numerators grow roughly like 2^{6n} while the denominators are $4\cdot 2^{12n}$.

b) Observe that formula (5.5.23) can be recast as

$$\frac{1}{\pi} = \frac{2\sqrt{2}}{9801}\sum_{n=0}^{\infty}\frac{(4n)!}{4^{4n}(n!)^4}[1103+26390n]\left(\frac{1}{99^4}\right)^n.$$

12. Use Exercise 6 of Section 1.3 to show that when $\operatorname{re}(c-a-b)>0$,

$${}_2F_1(a,b;c;1) = \frac{\Gamma(c)\Gamma(c-a-b)}{\Gamma(c-a)\Gamma(c-b)}.$$

[This is easy for $\operatorname{re}(c)>\operatorname{re}(b)>0$.]

13. Clausen's product formula is

$$[{}_2F_1(a,b;a+b+\tfrac{1}{2};z)]^2 = {}_3F_2(2a, a+b, 2b; a+b+\tfrac{1}{2}, 2a+2b; z).$$

Prove this by showing that both sides satisfy the same generalized hypergeometric equation and are analytic at zero, with value 1 there.

14. Verify that

a) $$\int_0^1\frac{K(k)\,dk}{\sqrt{1-k^2}} = \int_0^{\pi/2}\int_0^{\pi/2}\frac{d\alpha\,d\theta}{\sqrt{1-(\sin^2\alpha\sin^2\theta)}} = \frac{\pi^2}{4}\sum_{n=0}^{\infty}\left[\binom{2n}{n}4^{-n}\right]^3 = K^2\left(\frac{1}{\sqrt{2}}\right)$$

b) $$\frac{2}{\pi} = \lim_{t\to 1^-}\sqrt{(1-t)}\sum_{n=1}^{\infty}n\left[\binom{2n}{n}4^{-n}\right]^3 t^n.$$

15. Use Exercise 12 and Theorem 5.6(*ai*) to compute $K(1/\sqrt{2})$. Similarly use Theorem 5.6(*biv*) to compute $K(\sqrt{2}-1)$. (Compare Section 1.6.)

16. a) Verify that

i) $\sin(tx) = (t\sin x)\,{}_2F_1\left(\frac{1+t}{2}, \frac{1-t}{2}; \frac{3}{2}; \sin^2 x\right)$

ii) $\arcsin x = x\cdot {}_2F_1(\frac{1}{2}, \frac{1}{2}; \frac{3}{2}; x^2)$

iii) $\log(x+\sqrt{1+x^2}) = x\cdot {}_2F_1(\frac{1}{2}, \frac{1}{2}; \frac{3}{2}; -x^2)$.

b) Use Clausen's product to deduce that

$$\sin^2(t\sin^{-1}x) = -\frac{1}{2}\sum_{n=1}^{\infty}\frac{(t)_n(-t)_n}{(2n)!}(2x)^{2n}.$$

c) Similarly deduce Euler's formula (Bromwich [26])

$$\arcsin^2 x = \frac{1}{2}\sum_{n=1}^{\infty}\frac{(2x)^{2n}}{n^2\binom{2n}{n}}.$$

[This is also the limiting case of b). See also Exercise 16 of Section 11.3.]

d) Find similar formulae for $\sinh[t\log(x+\sqrt{1+x^2})]$ and for $\log(x+\sqrt{1+x^2})$.

e) Establish that

$$2\log^2\left(\frac{1+\sqrt{5}}{2}\right) = \sum_{n=1}^{\infty}\frac{(-1)^{n+1}}{n^2\binom{2n}{n}}$$

and that

$$\frac{\pi^2}{18} = \sum_{n=1}^{\infty}\frac{1}{n^2\binom{2n}{n}}.$$

f) Prove that

$$\frac{\sin(\pi t)}{\pi t} = \sum_{n=0}^{\infty}\frac{(t)_n(-t)_n}{(n!)^2}.$$

17. a) Prove that

$$\int_0^{1/2}\log^2(y+\sqrt{1+y^2})\frac{dy}{y} = \frac{1}{4}\sum_{n=1}^{\infty}\frac{(-1)^n}{n^3\binom{2n}{n}}.$$

b) Show that the previous integral is $\zeta(3)/10$. (See Exercises 12d) and 12e) of Section 11.3.)

18. Let $G_\alpha(x) := {}_2F_1(\alpha, (2\alpha+1)/2; 2\alpha+1; x)$.

a) From Clausen's product, establish that

$$G_{\alpha\beta} = G_\alpha^\beta \qquad \alpha, \beta \in \mathbb{R}.$$

b) Show that $G_{-1/2}(x) = (1+\sqrt{1-x})/2$. Thus

$$G_\alpha(x) := \left(\frac{1+\sqrt{1-x}}{2}\right)^{-2\alpha}.$$

(Note that $G_{-1/2}$ must be evaluated as a limit.)

19. a) Establish the solution of (5.5.28). *Hint*: $x := h'^2/h^2$ satisfies a simpler cubic than h^2.

b) Now verify that the following solutions obtain:

i) $G_3^{12} = 2$ gives $H_1^{24} = 1$

ii) $g_6^{12} = (\sqrt{2}+1)^2$ gives $H_2^{24} = 2$

iii) $G_9^{12} = (2+\sqrt{3})^2$ gives $H_3^{24} = \dfrac{2(2+\sqrt{3})^2}{3\sqrt{3}}$

iv) $g_{12}^{12} = \sqrt{2}(\sqrt{3}+1)^3$ gives $H_4^{24} = \dfrac{27}{2}$

v) $G_{15}^{12} = 8\left(\dfrac{\sqrt{5}+1}{2}\right)^4$ gives $H_5^{24} = \dfrac{125}{4}$

vi) $g_{18}^{12} = (\sqrt{3}+\sqrt{2})^4$ gives $H_6^{24} = \left(\dfrac{14\sqrt{3}+13\sqrt{2}}{3\sqrt{3}}\right)^2$.

Hint: For iii) and vi) use the increasing form of (5.5.28), which gives H_{3N} in terms of G_N. This entails changing the central sign in (5.5.28*ii*).

20. a) Establish the general formula for π^{-1} given by (5.5.33) and (5.3.34).

b) Verify the following values of $a_{1/6}(N) + nb_{1/6}(N)$:

i) $N := 2$ gives $(6n+1)/3\sqrt{3}$
ii) $N := 4$ gives $(60n+8)/27$
iii) $N := 5$ gives $(66n+8)/15\sqrt{3}$.

c) Compute the values of $a_{1/6}(N)$ and $b_{1/6}(N)$ for $N := 3$ and $N := 6$.

21. By comparing (5.5.33) with (5.5.16) or (5.5.18), verify the assertions of (5.5.31) for various N.

22. a) Use Exercise 12 to establish that

$$K_s\left(\frac{1}{\sqrt{2}}\right) = \frac{\Gamma(\frac14 + s/2)\Gamma(\frac14 - s/2)}{4\sqrt{\pi}} \cos(\pi s).$$

b) As in Exercise 15, compute $K(\lambda^*(3))$.

5.6 *OTHER APPROXIMATIONS*

We begin with equation (5.2.20), which we rewrite as

$$\sqrt{p}\left[1 - 24\sum_{n=1}^{\infty} \frac{n}{e^{2\pi\sqrt{p}n} - 1}\right] = \frac{3}{\pi} + \frac{\sigma(p)}{2}\left[\frac{2K(k)}{\pi}\right]^2 \tag{5.6.1}$$

where $k := \lambda^*(p)$. Then this shows that

$$\frac{3}{\pi} = \sqrt{p} - \frac{\sigma(p)}{2}\left[\frac{2K(k)}{\pi}\right]^2 + O(k^4\sqrt{p}). \tag{5.6.2}$$

Thus on approximating $2K/\pi$ by an algebraic quantity we produce various approximations for π. The simplest [which also follows from (5.2.15*i*)] is

$$\frac{3}{\pi} = \sqrt{p} - \frac{\sigma(p)}{2} + O(k^2\sqrt{p}). \tag{5.6.3}$$

We do better, however, by using Theorem 5.7(*a*) to write

$$\left[\frac{2K(k)}{\pi}\right]^2 = 1 + \frac{1}{2}(kk')^2 + O(k^4)$$

so that

$$\frac{3}{\pi} = \sqrt{p} - \frac{\sigma(p)}{4}[2 + (kk')^2] + O(k^4\sqrt{p}). \tag{5.6.4}$$

Ramanujan [14] uses different estimates of $2K/\pi$. Motivated perhaps by symmetry considerations, he uses (3.2.16) to expand $[2K(k)/\pi]^2$ as $(1-2k^2)^{-1} + O(k^2)$ and then (3.2.17) and (3.2.18) to obtain

$$\left[\frac{2K(k)}{\pi}\right]^2 = \frac{1-(kk')^2}{(1-2k^2)[1+\frac12(kk')^2]} + O(k^4).$$

Then his approximations to π are

(5.6.5) $$\pi_1(p) := \frac{3}{\sqrt{p} - \sigma(p)/[2(1-2k^2)]}$$

with error $O(\sqrt{p}e^{-\pi\sqrt{p}})$, and

(5.6.6) $$\pi_2(p) := \frac{3}{\sqrt{p} - [\sigma(p)(4G^{24}-1)]/[(1-2k^2)(8G^{24}+1)]}$$

with error $O(\sqrt{p}e^{-2\pi\sqrt{p}})$. (See Exercise 1.) Moreover, (5.6.5) and (5.6.6) produce very simple approximations. Thus

(5.6.7) $$\pi_1(25) = \frac{3(3+\sqrt{5})}{5} \quad \text{and} \quad \pi_2(25) = \frac{63(17+15\sqrt{5})}{25(7+15\sqrt{5})}.$$

The latter gives 11 digits of π. Similarly,

(5.6.8) $$\pi_1(37) = \frac{84}{21\sqrt{37}-101} \quad \text{and} \quad \pi_2(37) = 147\,\frac{145\sqrt{37}+1134}{22399\sqrt{37}-41916}.$$

(The values of α and σ are not quadratic surds.) For even p it is better to use

(5.6.9) $$\pi_3(p) = \frac{3}{\sqrt{p} - [\sigma(p)(4g^{24}+1)]/[(1+k^2)(8g^{24}-1)]}$$

which is again an $O(\sqrt{p}e^{-2\pi\sqrt{p}})$ approximation. Thus we derive

(5.6.10) $$\pi_3(22) = \frac{63\sqrt{22}(11+10\sqrt{2})}{887+1045\sqrt{2}}.$$

An even more classical approximation to π is obtained through taking logarithms of G_N or another invariant. Thus in the notation of the previous section we may write that π is approximately equal to

(5.6.11*i*) $$\frac{2}{\sqrt{N}}\log(8G_N^{12})$$

(5.6.11*ii*) $$\frac{2}{\sqrt{N}}\log(8g_N^{12})$$

or

(5.6.12*i*) $$\frac{2}{\sqrt{N}}\log\left(\frac{16}{y_N}\right)$$

(5.6.12*ii*) $$\frac{2}{\sqrt{N}}\log\left(\frac{16}{x_N}\right)$$

or

(5.6.13) $$\frac{1}{2\sqrt{N}}\log(1728J_N).$$

We leave it to the reader to estimate the error in each expression. (See Exercise 4.) For example, when $N := 58$, (5.6.11*ii*) produces

$$\frac{12}{\sqrt{58}}\log\left(\frac{\sqrt{29}+5}{\sqrt{2}}\right)$$

which gives 10 digits of π. Not surprisingly, Ramanujan [14] gives a host of examples of this kind. When the invariant is large these give very good algebraic approximations for e^{π}. Following Shanks [82] one can take this analysis considerably further. In (3.2.9) we gave q-product formulae for various invariants. Thus (3.1.4) and (3.2.9*ii*) yield

(5.6.14) $$x := f_1(\sqrt{-N})^{-24} = \left(\frac{k}{4k'^2}\right)^2 = q\prod_{n=1}^{\infty}(1+q^n)^{24}$$

and there is a similar expression for $(kk'/4)^2$. We may expand this product as a power series and compute as many terms as we wish of its reversion. This will produce a series of the form

(5.6.15) $$q = x - 24x^2 + 852x^3 - 35744x^4 + \cdots.$$

We may also take logarithms in (5.6.14). Then we can write

(5.6.16) $$\log x + \sqrt{N}\pi = 24\sum_{n=1}^{\infty}\log(1+q^n) = 24\sum_{k=1}^{\infty}\frac{(-1)^{k+1}}{k}q^k(1-q^k)^{-1}$$

which may be expanded as a power series in q. When we substitute (5.6.15) into (5.6.16) we will recursively compute

(5.6.17) $$\log(|x|) + \sqrt{N}\pi =: \sum_{n=1}^{\infty}(-1)^{n-1}\frac{a_n}{n}x^n$$

for a fixed sequence $\{a_n\}$. Indeed $a_1 := 1$, $a_2 := 47$, $a_3 := 2488$, $a_4 := 138799$, $a_5 := 7976456$, and $a_6 := 467232200$. In fact one can show (Newman and Shanks [84]) that $24a_n$ is the coefficient of q^n in $\prod_{k=1}^{\infty}(1+q^{2k-1})^{24n}$. Moreover, $24a_n < 64^n$. A now standard trick of replacing q by $-q$ shows that (5.6.17) still holds for $x := -(kk'/4)^2$. In Shanks [82] several large invariants are computed (including g_{3502} and G_{2737}) to which (5.6.17) may be applied.

Each series adds roughly $\pi\sqrt{N}\log_{10}e$ digits a term. Hence when we use g_{4698} given in (4.7.14), we gain more than 90 digits a term! But of course we have to compute the logarithm as well. Thus in our context the formula should be viewed as a rapid series for $\log(|x|)+\sqrt{N}\pi$, not as a computation of π.

Comments and Exercises

Approximations (5.6.5) and (5.6.6) were the reason why Ramanujan computed R_p. He did not give (5.6.9). Many very large invariants, including G_{14155}, G_{19947}, and G_{20155} are derived in Shanks [82].

1. a) Establish that (5.6.5) and (5.6.6) have the claimed errors without using the rather deep formulae (3.2.16) to (3.2.18).

b) Show, using (3.2.16) to (3.2.18), that

$$\pi_1(p)-\pi \sim 8\pi e^{-\pi\sqrt{p}}(\pi\sqrt{p}-3)$$

and

$$\pi_2(p)-\pi \sim 24\pi e^{-2\pi\sqrt{p}}(10\pi\sqrt{p}-31)\,.$$

2. a) Use (5.6.5) and (5.6.6.) to deduce that

$$\pi_1(13)=\frac{3(3\sqrt{13}+7)}{17} \quad\text{and}\quad \pi_2(13)=\frac{103\sqrt{13}+125}{158}\,.$$

b) Verify (5.6.7) and (5.6.8).

c) Verify that (5.6.9) has the claimed error.

d) Show that

$$\pi_1(93)=\frac{180+52\sqrt{3}}{45\sqrt{93}+39\sqrt{31}-201\sqrt{3}-217}\,.$$

3. a) For even p, the estimate

$$\pi_4(p):=\frac{3}{\sqrt{p}-\sigma(p)/2(1+k^2)}$$

will often be cleaner than $\pi_2(p)$. It also gives $O(\sqrt{p}e^{-\pi\sqrt{p}})$ error in estimation of π.

b) Obtain

$$\pi_4(58)=\frac{66\sqrt{2}}{33\sqrt{29}-148} \quad\text{and}\quad \pi_4(22)=\frac{6\sqrt{22}}{33-17\sqrt{2}}\,.$$

c) Compute $\pi_3(58)$ and $\pi_2(22)$.

4. a) Estimate the error in each of (5.6.11), (5.6.12), and (5.6.13). [Compare (2.5.15).]

b) Use (5.6.12) to estimate π by

$$\frac{4}{\sqrt{58}}\log(396) \quad\text{and}\quad \frac{4}{\sqrt{37}}\log(84\sqrt{2})\,.$$

5. a) Show that

$$g^{-24}=64q+1536q^2+19200q^3+\cdots$$

and

$$64g^{24}=q^{-1}-24+276q-2048q^2+\cdots$$

with similar expressions for G^{24}.

b) Thus

$$64(g_N^{24}+g_N^{-24})+24=e^{\pi\sqrt{N}}+4372e^{-\pi\sqrt{N}}+\cdots$$

and

$$64(G_N^{24}+G_N^{-24})-24=e^{\pi\sqrt{N}}+4372e^{-\pi\sqrt{N}}+\cdots\,.$$

c) When g_N or G_N is a quadratic surd, this gives an expression for the integer part of $e^{\pi\sqrt{N}}$ (and the proximate 0's or 9's). Thus the integer part of $e^{\pi\sqrt{22}}$ is 2,508,951. That of $e^{\pi\sqrt{37}}$ is 199,148,647, and that of $e^{\pi\sqrt{58}}$ is 24,591,257,751.

6. a) Show as discovered by Beukers that, with $\{a_n\}$ as in (5.6.17),

i) $$\left[\frac{\pi}{2K(k)}\right]^2=\sqrt{1-(2kk')^2}\left[1+24\sum_{n=1}^{\infty}a_n\left(\frac{kk'}{4}\right)^{2n}\right]$$

ii) $$\left[\frac{\pi}{2K(k)}\right]^2=(1+k^2)\left[1+24\sum_{n=1}^{\infty}(-1)^n a_n\left(\frac{k}{4k'^2}\right)^{2n}\right].$$

b) Combine *ai*) and Theorem 5.7(*ai*) to produce a recursion for $\{a_n\}$.

c) Show that a_n is an integer.

7. A variety of other approximations to π and to p, the perimeter of an ellipse, can be found in Chapter 18 of Ramanujan's second notebook and in Ramanujan [14]. For example, given an ellipse of major axis a, minor axis b, and eccentricity $k:=(b/a)'$, he gives

i) $$p=2\pi a\,{}_2F_1(\tfrac{1}{2},-\tfrac{1}{2};1;k^2)=\pi(a+b)\,{}_2F_1(-\tfrac{1}{2},-\tfrac{1}{2};1;t)$$

where $t:=[(a-b)/(a+b)]^2$. Then, as $t\to 0$,

ii) $p \sim \pi[3(a+b) - \sqrt{(3a+b)(3b+a)}]$

and

iii) $p \sim \pi(a+b)[1 + 3t(10 + \sqrt{4-3t})^{-1/2}]$

where the error in ii) is about $2^{-9}t^3$ and the error in iii) is about $3 \cdot 2^{-17}t^5$. This is pleasantly developed in Almqvist and Berndt [Pr] and in Berndt [Pr]. Truncating the approximation in iii) leads to

iv) $p \sim \pi(a+b)[1 + \frac{1}{8}t]^2$

with an error about $2^{-8}t^3$. This is due to Nyvoll [78].

a) Prove i).
b) Justify the error estimates in ii), iii), and iv).

One may avoid the Landen transform in a) by following Ivory [1796]. We write

$$p = 4aE(k) = 2a \int_0^\pi \left[1 - \frac{k^2}{2}(1 - \cos 2\theta)\right]^{1/2} d\theta$$

$$= (a+b) \int_0^\pi (1 + t^{1/2}e^{2i\theta})^{1/2}(1 + t^{1/2}e^{-2i\theta})^{1/2}\, d\theta$$

$$= (a+b) \sum_{m,n=0}^{\infty} (-1)^{m+n} \frac{(-\frac{1}{2})_m(-\frac{1}{2})_n}{m!n!} t^{(m+n)/2} \int_0^\pi e^{2i(m-n)\theta}\, d\theta .$$

8. a) Combine (5.1.2) and (5.2.14) to derive that

$$p = 4aE(k) \sim 2\pi a[M_n^{-1}(k,f) - M_n(k,f)\varepsilon_n(k,f)] \quad \text{as} \quad k \to 0$$

where $W_n(k^2, f^2) = 0$.

b) Show that the error is roughly of order ak^{2n}.

c) Deduce that to order ak^4,

$$p \sim 2\pi\left(\frac{a^2+b^2}{a+b}\right) \qquad n := 2$$

and to order ak^8,

$$p \sim 2\pi\left(\frac{a+b}{\sqrt{a}+\sqrt{b}}\right)^2 \qquad n := 4 .$$

d) Use the cubic identities to establish that

$$p \sim \pi a[3m^{-1}(r) + m(r) - 2]$$

when $k = \lambda^*(r)$. Thus, with order ak^6,

$k := \sqrt{2} - 1$ gives $2\pi a(5\sqrt{6} - 6\sqrt{3} - 7\sqrt{2} + 9)$

and $2kk' := \sqrt{5} - 2$ gives $\pi a[3(2+\sqrt{3})\sqrt{(2\sqrt{5} - 2\sqrt{3} - 1)} + \sqrt{(2\sqrt{5} + 2\sqrt{3} + 1)} - 2]$.

9. In the notation of the AGM iteration let $k := c_0/a_0$ and let $x_n^2 := c_{n+1}/a_{n+1}$.

a) Establish that

$$\sum_{n=1}^{\infty} \frac{1}{2^n} \log\left(\frac{1 + \sqrt{1 - x_n^4}}{2}\right) + \log\left(\frac{2}{x_1}\right) = \pi\, \frac{K'(k)}{K(k)} .$$

b) Let $x := (x_1/2)^4$ so that $x = [\frac{1}{2}(1 - \sqrt{k'})/(1 + \sqrt{k'})]^4$ and

$$\pi\, \frac{K'(k)}{K(k)} = -\frac{1}{4}\log x - 2x - \frac{26}{2}x^2 - \frac{368}{3}x^3 + \cdots .$$

c) Thus with $k := \lambda^*(r)$ one has another estimate for $\pi\sqrt{r}$ with x of order $e^{-4\pi\sqrt{r}}$. When $r := 1$, $x = \frac{1}{16}[(2^{1/4} - 1)^4/(2^{1/4} + 1)]^4$, and the given terms yield 19 digits of π.

From our point of view possibly the most remarkable result in Chapter 18 of Ramanujan's second notebook is the following continued fraction identity given in entry 12. Let $n > 0$ be fixed. Define

$$\Lambda_n(\alpha, \beta) := \frac{\alpha}{n+}\,\frac{\beta^2}{n+}\,\frac{(2\alpha)^2}{n+}\,\frac{(3\beta)^2}{n+}\,\frac{(4\alpha)^2}{n+}\cdots$$

for $\alpha, \beta > 0$. Then

(5.6.18) $$\Lambda_n\left(\frac{\alpha+\beta}{2}, \sqrt{\alpha\beta}\right) = \frac{\Lambda_n(\alpha,\beta) + \Lambda_n(\beta,\alpha)}{2}$$

whenever $\beta > \alpha > 0$ and

$$\mathrm{AG}(\beta, \sqrt{\beta^2 - \alpha^2}) = 1$$

[or, equivalently, whenever $K(\alpha/\beta) = (\pi/2)\beta$]. Even more surprisingly, a slight adjustment of the proof given in Berndt [Pr] shows that (5.6.18) holds for *all* $\alpha, \beta > 0$.

10. (*The moments of K and E*) Let

$$K_n := \int_0^1 k^n K(k)\, dk$$

and

$$E_n := \int_0^1 k^n E(k)\, dk\,.$$

a) Use the differential equations for K and E to establish that

$$K_{n+2} = \frac{nK_n + E_n}{n+2}$$

and

$$E_n = \frac{K_n + 1}{n+2}\,.$$

b) Show that

$$K_0 = \int_0^{\pi/2} \frac{\theta}{\sin\theta}\, d\theta = \sum_{n=0}^{\infty} \frac{1}{2n+1} \int_0^{\pi/2} \cos^{2n+1}\theta\, d\theta$$
$$= \sum_{n=0}^{\infty} \frac{4^n}{\binom{2n}{n}(2n+1)^2}\,.$$

c) Use contour integration of $\theta/\sin\theta$ (on the infinite rectangle above $[0, \pi/2]$) to deduce that

$$K_0 = 2\sum_{n=0}^{\infty} \frac{(-1)^n}{(2n+1)^2}$$

which is twice Catalan's constant, $\beta(2)$ or G.

d) Establish that $K_1 = 1$, $E_1 = \frac{2}{3}$, and $E_0 = \frac{1}{2} + \beta(2)$.

e) Observe that all the odd moments are rational while each even moment is of the form $a + b\beta(2)$ with a and b rational. Thus all moments lie in $\mathbb{Q}(\beta(2))$.

f) Analogously define K'_n and E'_n. Determine recursions for these conjugate moments. Show that $K'_0 = \pi^2/4$ and $E'_0 = \pi^2/8$. Compute K'_1 and E'_1.

g) Use the quadratic transformations to show that

$$\int_0^1 \frac{K(k)}{1+k}\, dk = \frac{1}{2} K'_0 = \frac{\pi^2}{8}\,.$$

h) Show that

$$\int_0^{\pi/6} \frac{\theta}{\sin\theta}\, d\theta = \frac{4}{3}\beta(2) - \frac{\pi}{6}\log(2+\sqrt{3})\,.$$

Chapter Six

The Complexity of Algebraic Functions

Abstract. *The aim of this chapter is to analyze the complexity of algebraic functions in general; and of multiplication, division, and root extraction in particular. There are two primary tools, Newton's method and the fast Fourier transform.*

6.1 COMPLEXITY CONCERNS

It is obviously inappropriate to consider the multiplication of two many-thousand-digit numbers to be of equal difficulty to the multiplication of two single-digit numbers. A reasonable measure of complexity that takes this into account is the bit complexity. The *bit complexity* of an algorithm is the number of single-digit operations required to terminate the algorithm. Single-digit operations include addition, multiplication, logical comparison, and storage and retrieval of single-digit numbers. We are exclusively interested in how the complexity increases with the size of the problem. For example, addition of two n-digit integers by the usual algorithm has bit complexity $O_B(n)$—the subscript B on the order symbol is for emphasis. This is a serial notion of complexity in the sense that on a serial machine it is an appropriate asymptotic measure of the time required for the calculation. We use the slightly nonstandard notation

$$a_n = \Omega(b_n)$$

if

$$a_n = O(b_n) \quad \text{and} \quad b_n = O(a_n)\,.$$

If $a_n = \Omega(b_n)$, we say that $\{a_n\}$ and $\{b_n\}$ are equivalent. Since accessing an n-digit number requires $\Omega(n)$ bit operations, it is apparent that "usual" addition of two n-digit integers is in fact $\Omega(n)$. These trivial lower bounds are a consequence of uniqueness considerations—if we change any digit of one of the numbers being added, we change the answer. Thus any algorithm for addition must at least "inspect" every digit. So, up to a constant, usual additon is asymptotically optimal. As we shall see later, one of the interesting consequences of this body of theory is that "usual" multiplication is far from asymptotically optimal.

A detailed approach to complexity requires a model of computation and is perhaps most readily made rigorous in an analysis of Turing machines. (See, for example, Aho, Hopcroft, and Ullman [74].) This much detail is unnecessary for our purposes.

We will usually content ourselves with merely counting single-digit additions and multiplications. In all the algorithms we present the comparisons [note that the comparison of two n-digit numbers is $\Omega_B(n)$] and the storage concerns will be bounded by the arithmetic operations—provided the algorithms are sensibly implemented. This is almost always transparent and will rarely even elicit comment.

Operational complexity counts the number of operations (addition, multiplication, division, and extraction of kth roots performed to a precision bounded by the precision of the output). When all the operations in an algorithm are performed to roughly the same precision, this is a useful measure. The reasons for the particular choice of operations will be made apparent in Section 6.4. Thus the algorithms of Chapter 5 compute n digits of π with operational complexity $O_{\mathrm{op}}(\log n)$; once again the subscript on the order symbol is for emphasis.

Comments and Exercises

One of the primary tools for the analysis of algorithms is the use of recursive functions. The idea is to divide a problem into smaller subproblems that can be solved by essentially the same technique and then recurse, a strategy often called "divide and conquer." The reader unfamiliar with this approach might like to examine the exercises. One of the lessons of complexity theory is that many of the usual algorithms of mathematics are far from optimal. Multiplication, taking Fourier transforms, and matrix multiplication are but three examples. (See Exercise 3 and the next section.) A second lesson is that good lower bounds are very difficult to obtain. For the analytic algorithms we are considering, the only lower bounds we can establish are the trivial ones. Thus unless the algorithm is of the same order, as is the case for addition, we cannot achieve exact results.

We shall not discuss combinatorial complexity except to mention that an introduction to this well-developed and important field may be found in Aho, Hopcroft, and Ullman [74].

1. Prove the following. Let $a, b > 0$ and $c > 1$. Suppose that f is monotone on $(0, \infty)$.

   a) If $f(n) < af(n/c) + bn$ and $f(1) = d$, then

$$\begin{aligned} f(n) &= O(n) && \text{if } a < c \\ f(n) &= O(n \log n) && \text{if } a = c \\ f(n) &= O(n^{\log_c a}) && \text{if } a > c\,. \end{aligned}$$

   b) If $f(n) \le af(n/a) + bn(\log n)^{c-1}$ and $f(1) = d$, then

$$f(n) = O(n(\log n)^c)\,.$$

   Hint: Analyze a) with equality. Then establish the general principle that the equality solution is the maximal solution.

2. Show that the usual algorithms for multiplying and adding two $n \times n$ matrices have complexity $\Omega_{\mathrm{op}}(n^3)$ and $\Omega_{\mathrm{op}}(n^2)$, respectively. (We are counting the number of multiplications and additions of the entries of the matrices.)

3. (*Fast matrix multiplication* (*Strassen* 1969))

   a) Show that

$$\begin{bmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{bmatrix}\begin{bmatrix} B_{11} & B_{12} \\ B_{21} & B_{22} \end{bmatrix} = \begin{bmatrix} C_{11} & C_{12} \\ C_{21} & C_{22} \end{bmatrix}$$

   can be computed from

$$\begin{aligned} M_1 &= (A_{12} - A_{22})(B_{21} + B_{22}) \\ M_2 &= (A_{11} + A_{22})(B_{11} + B_{22}) \\ M_3 &= (A_{11} - A_{21})(B_{11} + B_{12}) \\ M_4 &= (A_{11} + A_{12})B_{22} \\ M_5 &= A_{11}(B_{12} - B_{22}) \\ M_6 &= A_{22}(B_{21} - B_{11}) \\ M_7 &= (A_{21} + A_{22})B_{11} \end{aligned}$$

   and

$$\begin{aligned} C_{11} &= M_1 + M_2 - M_4 + M_6 \\ C_{12} &= M_4 + M_5 \\ C_{21} &= M_6 + M_7 \\ C_{22} &= M_2 - M_3 + M_5 - M_7\,. \end{aligned}$$

   b) Observe that the above method reduces the multiplication of $2n \times 2n$ matrices to 7 multiplications and 18 additions of $n \times n$

matrices. Thus if $W(n)$ is the operational complexity of multiplying two $n \times n$ matrices, then by iterating the procedure in a)

$$W(2n) \le 7W(n) + \alpha n^2\,.$$

The final term comes from using usual matrix addition for the 18 additions. The constant α can be chosen independent of n and can be used to include the "overhead" of actually breaking the problem up. Use the above inequality to show that

$$W(n) = O_{\mathrm{op}}(n^{\log_2 7})\,.$$

Note that $\log_2 7 \le 2.81$, so the above method is asymptotically faster than the usual method. [Extensions of this method can reduce the bound for multiplication down at least to $O(n^{2.5-})$, much as in Knuth [81]. The best lower bound known is the trivial one, cn^2.]

4. Suppose A is a nonsingular $2n \times 2n$ triangular matrix. Write

$$A = \begin{pmatrix} B & 0 \\ C & D \end{pmatrix}$$

where B, C, and D are $n \times n$ matrices.

   a) Show that B^{-1} and D^{-1} exist, and that

$$A^{-1} = \begin{pmatrix} B^{-1} & 0 \\ -D^{-1}CB^{-1} & D^{-1} \end{pmatrix}.$$

   b) Show that a) iterates to produce an algorithm for inverting $2^m \times 2^m$ triangular matrices. Let $I(n)$ be the operational complexity of this algorithm. Show with $W(n)$ as in Exercise 3 that

$$I(2n) \le 2W(n) + 2I(n) + cn^2$$

   and hence that

$$I(n) = O(W(n)) = O(n^{\log_2 7})\,.$$

   (One can show that in general matrix inversion and matrix multiplication are asymptotically equivalent. See Aho, Hopcroft, and Ullman [74].)

5. Show that the bit complexity of calculating $n!$ by multiplying $1 \times 2 \times 3 \times \cdots$ using usual multiplication is $\Omega((n \log n)^2)$.
   Hint: Analyze the complexity of multiplying an n-digit number by an m-digit number. Use Stirling's formula to estimate the number of digits in $k!$. Exercise 10 of Section 6.4 explores this further.

6.2 THE FAST FOURIER TRANSFORM (FFT)

Let w be a primitive $(n+1)$th root of unity either in $\mathbb{C}$ or in a finite field F_m, that is, $w^{n+1}=1$ and $w^k \neq 1$ for $k<n+1$. In the complex case we may take $w := e^{2\pi i/(n+1)}$. Consider the following two problems.

INTERPOLATION PROBLEM. Given $n+1$ numbers $\alpha_0, \ldots, \alpha_n$, find the coefficients of the unique polynomial $p_n(z) := a_0 + a_1 z + \cdots + a_n z^n$ of degree n that satisfies

$$p_n(w^i) = \alpha_i \qquad 0 \le i < n+1 .$$

EVALUATION PROBLEM. Given the coefficients of a polynomial p_n of degree n, calculate the $n+1$ values

$$p_n(w^i) \qquad 0 \le i < n+1 .$$

These are the two directions of the *finite* or *discrete Fourier transform*. The classical approaches to either part of the Fourier transform problem have operational complexity at least cn^2. This is the operational complexity, for example, of evaluating p_n at $n+1$ points using *Horner's rule* [writing $p_n(x) = (((a_n x + a_{n-1})x + a_{n-2})x + \cdots)$]. We wish to prove that, in fact, both directions can be solved with complexity $O_{\mathrm{op}}(n \log n)$. Actually, we only treat the case $n+1 := c2^m$, which is sufficient for our purposes and somewhat simpler.

Theorem 6.1 ***(Fast Fourier Transform)***

If $n+1 = c2^m$ with c an integral constant, then both the interpolation and the evaluation problem have operational complexity $O_{\mathrm{op}}(n \log n)$.

Proof. We assume $c=1$, that is, $n+1=2^m$, the case for general c is entirely analogous. We treat evaluation first. Suppose

$$p(x) := a_0 + \cdots + a_n x^n .$$

Let

$$q(x^2) := a_0 + a_2 x^2 + a_4 x^4 + \cdots + a_{n-1} x^{n-1}$$

and

$$xr(x^2) := x(a_1 + a_3 x^2 + \cdots + a_n x^{n-1}) .$$

Then with $y := x^2$,

$$p(x) = xr(y) + q(y) \tag{6.2.1}$$

where r and q are both polynomials of degree $2^{m-1}-1$. The observation that makes the proof work is that for w an $(n+1)$th root of unity,

$$(w^i)^2 = (w^{(n+1)/2+i})^2 .$$

Hence, evaluating $p(x)$ at the $n+1$ roots of unity in (6.2.1) reduces to evaluating r and q each at the $(n+1)/2$ points $(w^2)^1, (w^2)^2, \ldots, (w^2)^{(n+1)/2}$ and amalgamating the results. Observe that w^2 is a primitive (2^{m-1})th root of unity and we can iterate this process. Let $F(2^m)$ be the number of additions and multiplications required to evaluate a polynomial of degree 2^m-1 at the 2^m points w^k, $k=1,\ldots,2^m$, where w is a primitive (2^m)th root of unity. As above,

$$F(2^m) = 2F(2^{m-1}) + 2\cdot 2^m \qquad F(1)=0 . \tag{6.2.2}$$

The final term comes from the single addition and multiplication required to calculate each $p(w^i)$ from $r(w^{2i})$ and $q(w^{2i})$. The recursion (6.2.2) solves as

$$F(2^m) = 2^{m+1}\cdot m \tag{6.2.3}$$

and the bound for the evaluation problem follows.

The interpolation problem is equivalent to evaluation. This can be seen as follows. Let w be a primitive $(n+1)$th root of unity and let

$$W := \begin{pmatrix} 1 & 1 & 1 & \cdots & 1 \\ 1 & w & w^2 & \cdots & w^n \\ 1 & w^2 & w^4 & \cdots & w^{2n} \\ \vdots & & & & \vdots \\ 1 & w^n & w^{2n} & \cdots & w^{n^2} \end{pmatrix} . \tag{6.2.4}$$

Then

$$W^{-1} = \frac{1}{n+1}\begin{pmatrix} 1 & 1 & 1 & \cdots & 1 \\ 1 & w^{-1} & w^{-2} & \cdots & w^{-n} \\ 1 & w^{-2} & w^{-4} & \cdots & w^{-2n} \\ \vdots & & & & \vdots \\ 1 & w^{-n} & w^{-2n} & \cdots & w^{-n^2} \end{pmatrix} \tag{6.2.5}$$

and w^{-1} is also a primitive $(n+1)$th root of unity. (See Exercise 4.) The interpolation problem can be written as: Find $(a_0, \ldots, a_n)$ so that

$$W(a_0, \ldots, a_n) = (\alpha_0, \ldots, \alpha_n) .$$

However, this can be solved by

$$W^{-1}(\alpha_0, \ldots, \alpha_n) = (a_0, \ldots, a_n)$$

which is exactly the evaluation problem. □

While restricting the FFT to powers of 2 poses no problem for us over $\mathbb{C}$, it is a nuisance over finite fields. The problem is that F_m has primitive kth roots if and only if k divides $m-1$. Hence, our approach is restricted in the finite case to considering primes of the form $m = c2^k + 1$, which are not particularly abundant. There are many ways around this difficulty. This is discussed in Winograd [80].

Comments and Exercises

The FFT is an enormously useful and widely used algorithm. Depending on exact form and implementation, it can outperform traditional methods for values of n well below 100. For a history of the FFT consult Cooley, Lewis, and Welch [67]. While antecedents for FFT methods are plentiful, Cooley and Tukey [65] are primarily responsible for introducing the FFT in its modern form as a complexity-reduced method. More extended disucssion of the FFT and related matters may be found in Aho, Hopcroft, and Ullman [74] and Winograd [80]. As a theoretical tool the FFT and related methods are central. They form the basis for the next section's discussion of fast multiplication. In the exercises we show how these ideas can be used to construct asymptotically fast polynomial multiplication, division, and interpolation algorithms. It is even possible to accelerate integer factoring algorithms by FFT methods. In Chapter 10 an application to the estimation of certain transcendental functions is provided. Our proof of Theorem 6.1 and some of the exercises follow Borodin and Munro [75].

1. a) (*Fast polynomial multiplication*) Consider the following algorithm for multiplying polynomials. Given the coefficients of p and q (both of degree $\le n-1$), compute the coefficients of pq as follows:

Step 1: Evaluate p and q at $2n$ points $w^1, \ldots, w^{2n}$, where w is a primitive $(2n)$th root of unity.*

Step 2: Form the $2n$ products

$$p(w^i)q(w^i) \qquad i = 1, \ldots, 2n.$$

Step 3: Solve the interpolation problem for pq to find the coefficients.

Show, using an FFT, that the above algorithm has operational complexity

$$O_{\text{op}}(n \log n).$$

[The usual convolution product algorithm has operational complexity $\Omega(n^2)$.]

b) Given

$$p(x) := \prod_{i=1}^{n} (x - x_i)$$

show that the coefficients of p can be calculated in $O_{\text{op}}(n(\log n)^2)$. *Hint*: Treat the problem recursively and recombine the pieces using a fast polynomial multiplication.

2. (*Fast polynomial division*) Given p of degree n and q of degree $m \le n$, both with integer coefficients, it is possible to find u and r with $\deg r < \deg q$ so that

$$p(x) = u(x)q(x) + r(x)$$

in $O_{\text{op}}(n \log n)$.

Outline: Simplify by observing that it suffices to calculate u since r may then be computed by Exercise 1. Set $x := 1/x$. Then

$$\frac{p(1/x)}{q(1/x)} = u\left(\frac{1}{x}\right) + \frac{r(1/x)}{q(1/x)}$$

and so

$$\frac{\bar{p}(x)}{\bar{q}(x)} = \bar{u}(x) + x^{n-m+h}\,\frac{\bar{r}(x)}{\bar{q}(x)} \qquad \bar{v}(x) := x^{\deg v}\, v\left(\frac{1}{x}\right)$$

where $h \ge 1$. To calculate $\bar{u}$ (and hence u) it suffices to calculate the first $n-m$ $(=\deg u)$ Taylor coefficients of $1/\bar{q}$. This can be done by Newton's method as follows. Suppose that $\deg s_i = j-1$ and that

$$\frac{1}{\bar{q}(x)} - s_i(x) = O(x^j).$$

Establish that

$$\frac{1}{\bar{q}(x)} - [2s_i(x) - s_i^2(x)\bar{q}(x)] = \frac{1}{\bar{q}(x)}\,[1 - s_i(x)\bar{q}(x)]^2 = O(x^{2j}).$$

[Note that we may assume $\bar{q}(0) \ne 0$.] Now the computation of $s_{i+1} := 2s_i - s_i^2\bar{q}$ can be performed using an FFT-based polynomial multiplication and need only be performed using the first $2j-1$ coefficients of $\bar{q}$ and s_i. By starting with an appropriate first estimate of s_0 [say, $s_0(x) := 1/\bar{q}(0)$] and proceeding inductively as above (doubling the number of coefficients utilized at each stage), show that the required number of terms of the expansion can be calculated in $O_{\text{op}}(n \log n)$. (See Section 6.4.)

* Strictly speaking, we should be using (2^m)th roots of unity where we have established an FFT. This can be arranged by padding with leading zero terms, if necessary, without changing the order of complexity.

3. (*Fast polynomial evaluation*) Given p of degree n and $n+1$ distinct points $x_0, \ldots, x_n$, show that $p(x_0), \ldots, p(x_n)$ can all be evaluated in $O_{op}(n(\log n)^2)$.
Hint: Let $q_1(x) = \Pi_{i=0}^{n/2-1}(x - x_i)$ and let r_1 be the remainder on dividing p by q_1. Note that $r_1(x_i) = p(x_i)$ for $i < n/2$. Similarly use $q_2(x) := \Pi_{n/2}^{n}(x - x_i)$. Thus two divisions reduces the problem to two problems of half the size. Use Exercise 2 and evaluate the recursion. [The other direction of this problem, namely, constructing Lagrange interpolating polynomials, is also $O_{op}(n(\log n)^2)$. See, for example, Borodin and Munro [75]. In fact, both directions are $\Omega_{op}(n \log n)$.]

4. Show that if w is a primitive $(n+1)$th root of unity, then

$$\sum_{i=0}^{n} w^{ij} = \begin{cases} n+1 & j \equiv 0 \bmod (n+1) \\ 0 & \text{otherwise}. \end{cases}$$

Show that (6.2.4) and (6.2.5) are inverse to each other.

5. (*Reversion of power series*) Let $f(x) := \Sigma_{k=0}^{\infty} a_k x^k$ be a formal power series, with known coefficients.

a) Show, as in the proof of Exercise 2, that the first n coefficients of the formal series expansion of $1/f(x)$ can be computed in $O_{op}(n \log n)$.
b) Discuss the complexity of computing the coefficients of the formal inverse of f by Newton's method.

6. (*On calculating* x^n) The S-and-X binary method for calculating x^n is the following rule. Suppose n has binary representation $\delta_0\delta_1\delta_2 \cdots \delta_k$ with $\delta_0 = 1$. Given symbols S and X, define

$$S_i := \begin{cases} SX & \text{if } \delta_i = 1 \\ S & \text{if } \delta_i = 0 \end{cases}$$

and construct the sequence

$$S_1 S_2 \cdots S_k.$$

Now let S be the operation of squaring and let X be the operation of multiplying by x. Let the sequence of operations $S_1S_2 \cdots S_k$ operate from left to right beginning with x. For example, for $n = 27$,

$$\delta_0\delta_1\delta_2\delta_3\delta_4 = 11011$$

and

$$S_1S_2S_3S_4 = (SX)(S)(SX)(SX).$$

The sequence of calculations for x^{27} is then

$$x \to x^2 \to x^3 \to x^6 \to x^{12} \to x^{13} \to x^{26} \to x^{27}.$$

a) Prove that the above method computes x^n and observe that it only requires storing x, n, and one partial product.
b) Show that the number of multiplications is less than $2\lfloor \log_2 n \rfloor$.
c) Show that the above method is optimal for the computation of x^{2^m} (considering only multiplications).
d) Show that the S-and-X method is not optimal for computing x^{15}.

An extended discussion of this interesting and old problem is presented in Knuth [81].

6.3 *FAST MULTIPLICATION*

We wish to present a strategy for multiplying very large numbers that is considerably faster than the usual $O_B(n^2)$ method. The idea is to exploit the FFT. Let α and β be two n-digit integers and write

$$\alpha(x) := a_n x^{n-1} + a_{n-1} x^{n-2} + \cdots + a_1 \tag{6.3.1}$$

and

$$\beta(x) := b_n x^{n-1} + b_{n-1} x^{n-2} + \cdots + b_1. \tag{6.3.2}$$

Then if a_i and b_i are the decimal digits of α and β, respectively, we have

$$\alpha = \alpha(10) \quad \text{and} \quad \beta = \beta(10). \tag{6.3.3}$$

We can now calculate $\alpha \cdot \beta$ by using the FFT, as in Exercise 1 of the last section, to compute the coefficients of

$$\gamma(x) := \alpha(x)\beta(x). \tag{6.3.4}$$

Finally we evaluate $\gamma(10)$.

Let $T(n)$ denote the bit complexity of multiplying two n-digit integers (or equivalently, floating point numbers) by the above method.

The analysis of the complexity of the algorithm that follows assumes that we are working with complex roots of unity (and that we are working with a problem of size 2^m, as can always be arranged by padding with leading zeros). This introduces rounding error problems into an intrinsically integer algorithm; however, this is the setting which we have established an abundance of values for which the FFT works. Since in practice (and in theory) there are plenty of FFT analogues in a finite setting, one may, if one prefers, consider the entire algorithm performed mod $(O(n))$.

Step 1: Evaluate $\alpha(x)$ and $\beta(x)$ to precision $O(\log n)$ at the $2n$ points $w^1, w^2, \ldots, w^{2n}$ with w a primitive $(2n)$th root of unity. Using the FFT, this has operational complexity

$$O_{\text{op}}(n \log n)$$

and bit complexity

$$O_B(n(\log n)T(\log n)) . \tag{6.3.5}$$

[It suffices to use w to precision $O(\log n)$ and thus every multiplication in Theorem 6.1 is of complexity $O_B(T(\log n))$. Observe that the coefficients of α and β are single-digit numbers and that the coefficients of γ are hence $O(\log n)$-digit numbers. See Exercise 3.]

Step 2: Form the $2n$ products

$$\gamma(w^i) = \alpha(w^i)\beta(w^i)$$

computed to $O(\log n)$ digit precision. This is of bit complexity

$$O_B(nT(\log n)) . \tag{6.3.6}$$

Step 3: Interpolate the coefficients of γ to precision $O(\log n)$ using the FFT. This has operational complexity

$$O_{\text{op}}(n \log n)$$

and bit complexity, as before,

$$O_B(n(\log n)T(\log n)) . \tag{6.3.7}$$

Step 4: Evaluate $\gamma(10)$. This has bit complexity

$$O_B(n) . \tag{6.3.8}$$

This step essentially requires only addition. The coefficients of γ are closely related to the digits of $\alpha\beta$ except that they may be too large and a "carry" must be performed.

The total complexity thus satisfies

$$T(n) = O_B(n(\log n)T(\log n)) \tag{6.3.9}$$

or

$$T(n) = O_B(n(\log n)^2(\log(\log n))^2 \cdots) \tag{6.3.10}$$

with the product terminating when the iterated log is less than 1.

This is not optimal. (See Exercise 2.) The same analysis as above using a base n representation of α and β reduces the time for multiplication to

$$O_B(n(\log n)(\log\log n) \cdots) .$$

This is still not quite the asymptotically fastest known algorithm. The best bound is due to Schönhage and Strassen [71] and is

$$O_B(n(\log n)(\log\log n)) .$$

We shall call any multiplication that performs with this speed a *Schönhage–Strassen multiplication*. It should be emphasized that in all the reduced complexity multiplications we present, the order estimates include the overhead additions (and storage concerns).

Comments and Exercises

The observation that multiplication is not intrinsically $O_B(n^2)$ was made by Karatsuba in 1962. He proposed an $O_B(n^{\log_2 3})$ algorithm. (See Exercise 1.) Subsequent refinements and improvements are due to Toom, Cook, Schönhage, Strassen, and others, culminating in the Schönhage–Strassen multiplication of 1971. This algorithm is of the same flavour as the one presented above using size $2^{\sqrt{n}}$ representations and performing FFT operations mod$(2^{2\sqrt{n}}+1)$. A presentation may be found in Aho, Hopcroft, and Ullman [74]. Knuth [81] has an extended discussion of multiplication strategies which includes a discussion of the precision concerns of performing a fast multiplication over $\mathbb{C}$. Cook and Aanderaa [69] conjecture that multiplication is not $O_B(n)$. Here one must be careful about the model of computation allowed. Under some more powerful than usual models $O_B(n)$ multiplication is possible (see Knuth [81]), while under other more restrictive than usual models it can be shown to be not possible.

Once again it is possible to implement a fast multiplication that will outperform traditional methods for n in the several hundred-digit range. For the many million-digit calculations of π discussed in Chapter 11, use of a fast multiplication is imperative. For a discussion of the multiplication used in this setting see Tamura and Kanada [Pr] and Bailey [Pr].

1. (*An* $O_B(n^{\log_2 3})$ *multiplication*) Observe that

$$(a + b10^n)(c + d10^n) = ac + [(a - b)(d - c) + ac + bd]10^n + bd10^{2n}.$$

Use this to reduce multiplication of $2n$-digit numbers to three multiplications of n-digit numbers and some additions. Show that this can be used to produce a multiplication of

$$O_B(n^{\log_2 3}).$$

[This method can be refined to produce an $O_B(n^{1+\delta})$ algorithm; details are in Knuth [81].]

2. Construct a multiplication of complexity

$$O_B(n(\log n)(\log\log n)\cdots).$$

Hint: Instead of using base 10 representations, use base n representations so that the polynomials (6.3.1) and (6.3.2) are polynomials of degree n with coefficients of length $\log n$. Now proceed as in the algorithm of this section.

3. Discuss the bit complexity of the FFT. Show that if the input is given to precision $O(m)$ and the output is required to precision $O(m)$, the bit complexity is

$$O_B((n \log n)M(m))$$

where $M(m)$ is the complexity of whatever multiplication is employed.

6.4 NEWTON'S METHOD AND THE COMPLEXITY OF ALGEBRAIC FUNCTIONS

We wish to show the equivalence, from a complexity point of view, of multiplication, division, and root extraction. The primary tool is Newton's method.

Theorem 6.2

Suppose that f is analytic in a complex neighbourhood of z. Suppose $f(z) = 0$ and $\dot{f}(z) \neq 0$. Then the iteration

$$x_{n+1} := x_n - \frac{f(x_n)}{\dot{f}(x_n)} \qquad (6.4.1)$$

converges uniformly quadratically to z for initial values x_0 in some neighbourhood of z.

The reader unfamiliar with the proof is directed to Exercise 1. Newton's method is useful for calculating inverse functions. Observe that $g^{-1}(y)$ is a zero of $f(x) = g(x) - y$. This is the content of the corollary. The uniform nature of the convergence is discussed in the exercises.

Corollary 6.1

Suppose that f is analytic and one to one in a neighbourhood of z_0. Then there is a neighbourhood of $f(z_0)$ where f^{-1} can be computed uniformly quadratically by Newton's method.

The quadratic nature of the convergence is only half the story. The other half is the "self-correcting" nature of Newton's method. Suppose that $f(z) = 0$ and that we are computing z by Newton's method. If the nth iterate x_n is perturbed by an amount $O(|x_n - z|)$, then provided we stay in the domain of uniform quadratic convergence, computing x_{n+1} from the perturbed value of x_n will preserve quadratic convergence. In other words, if $x_n - z$ agree through M digits, then the calculation of x_{n+1} need only be performed to precision $2M$.

Let $M(n)$ denote the bit complexity of multiplication of two n-digit numbers by some method. We make the following regularity assumptions:

$$2M(n) \le M(2n) \le 4M(n) \quad \text{and} \quad M(n) \text{ is nondecreasing}. \qquad (6.4.2)$$

Since two multiplications of length n can be viewed as subproducts of a single multiplication of length $2n$, while four multiplications of length n comprise one of length $2n$, the first part of the assumption is reasonable. Since multiplications of length n can be padded with leading zeros to multiplications of length $n + k$, the second part is also reasonable. Of course it is easy to imagine a perversely designed multiplication for which (6.4.2) does not hold.

Let $D(n)$ and $R(n)$, respectively, denote the bit complexity of division and extraction of square roots, where the input and output are to precision n. We say that two operations are *equivalent* if the complexity of one is bounded by the complexity of the other and conversely. For example, we say multiplication and division are equivalent if, given a multiplication with bit complexity $M(n)$, we can construct a division with bit complexity $D(n) = O(M(n))$; and conversely, given a division we can so construct a multiplication. The following remarkable theorem, the first part of which is due to Cook, may be found in Brent [76c].

Theorem 6.3

Multiplication, division, and root extraction are all equivalent.

Proof.

(*a*) We first construct a division. Applying Newton's method to the function $f(x) := 1/x - y$ leads to the iteration

$$x_{k+1} := 2x_k - x_k^2 y \tag{6.4.3}$$

which employs only multiplication and addition. Note that

$$x_{k+1} - \frac{1}{y} = -y\left(x_k - \frac{1}{y}\right)^2 \tag{6.4.4}$$

and the quadratic nature of the convergence is manifest. We assume $|y| \le 1$ and that y lies in a neighbourhood V bounded away from zero (which if we are working in floating point, is no restriction). We may also assume that, by using a usual $O_B(n^2)$ division performed to a fixed low precision, we have already computed $x_0 := x_0(y)$, so that $|x_0 - 1/y| < 1/10$. Assume n is a power of 2. Then $\log_2 n$ iterations of (6.4.3) will by (6.4.4) produce an error bounded by

$$\left|\left(x_0 - \frac{1}{y}\right)^n\right| \le 10^{-n}$$

and hence provide n digits of $1/y$. Furthermore, by the self-correcting nature of Newton's method, the kth step of (6.4.3) requires two multiplications and two additions of precision only 2^k. Thus the total complexity of the iteration is given by

$$\sum_{k=1}^{\log_2 n} [2M(2^k) + 2 \cdot 2^k] \le 8M(n) \tag{6.4.5}$$

since $2M(2^k) \le M(2^{k+1})$. We have shown that $1/y$ can be calculated with complexity $O_B(M(n))$. Hence since $a/b = a \cdot (1/b)$,

$$D(n) = O_B(M(n))\ .$$

(*b*) The equivalence of division and multiplication is now obvious since

$$ab = \frac{a}{1/b}\ .$$

(*c*) Square roots can be extracted by Newton's method applied to $x^2 - y$, which yields the classical iteration

$$x_{k+1} := \frac{1}{2}\left(x_k + \frac{y}{x_k}\right). \tag{6.4.6}$$

This satisfies

$$x_{k+1} - \sqrt{y} = \frac{1}{2x_k}(x_k - \sqrt{y})^2 \tag{6.4.7}$$

and the quadratic convergence is again apparent. We can proceed exactly as in (*a*) to show that

$$R(n) = O_B(D(n)) = O_B(M(n))\ .$$

(*d*) The proof that

$$M(n) = O_B(R(n))$$

is Exercise 7. □

It is apparent that any time a function may be quadratically computed by Newton's method from an iteration involving only addition, multiplication, and division, that function will be of complexity $O_B(M(n))$. This applies to any algebraic function over $\mathbb{Q}(x)$, that is, any function f satisfying an equation

$$\Phi(x, f(x)) = 0 \tag{6.4.8}$$

where Φ is a polynomial in two variables with rational coefficients. More precisely:

Theorem 6.4

If f is algebraic over $\mathbb{Q}(x)$, then the complexity of calculating n digits of $f(x)$ is $O_B(M(n))$.

The preceding results, of course, assume that we are avoiding the branch points of the function in question.

Comments and Exercises

Newton's method has a host of refinements and variants. See, for example, Householder [70] and Exercise 3. The iteration for square roots can in some form be traced back to the Babylonians, who used one or two steps of the method.

It should be observed that not only is $D(n) = O_B(M(n))$, but the constant concealed by the order sign is fairly small. [From (6.4.5) we see that a constant 8 works. Indeed, for all known multiplications, the additions term is negligible and a constant of 4 is appropriate.] This is also the case for root extraction. See Brent [76c], where a number of constants for these and various other equivalences, as in Exercise 7, are established.

Further discussion of the calculation of algebraic functions may be found in Kung and Traub [78]. Related matters may also be pursued in Lipson [81].

1. a) Prove Theorem 6.1 by observing that

$$f(x_n) = f(z) + (x_n - z)\dot{f}(z) + O(x_n - z)^2 .$$

Substitute this into (6.4.1) to get

$$x_{n+1} - z = (x_n - z)\left[\frac{\dot{f}(x_n) - \dot{f}(z)}{\dot{f}(x_n)}\right] + O(x_n - z)^2 .$$

Use explicit estimates to prove uniformity.

b) Show that for real f and real x_n, the tangent to f at x_n intersects the x axis at x_{n+1}.

c) Suppose that f is convex and strictly increasing on $[a, b]$ and that $f(\bar{x}) = 0$ for some $\bar{x}$ in (a, b). Show that if $b \geq x_0 > \bar{x}$, then $\{x_n\}$ decreases to $\bar{x}$ and convergence is guaranteed.

2. Construct the Newton iteration for $y^{1/p}$ by inverting x^p. Write $x_{n+1} - y^{1/p}$ in terms of $(x_n - y^{1/p})^2$, thus exhibiting explicitly the quadratic convergence. For which real starting values does the method converge?

3. a) Consider the iteration

$$y_{k+1} = y_k + (n+1)\left.\frac{(1/f)^{(n)}}{(1/f)^{(n+1)}}\right|_{y_k}$$

where the notation indicates that the derivatives are evaluated at y_k. For sufficiently well-behaved (for example, analytic) f, this method will find a zero of f with $(n+2)$th-order convergence provided various derivatives are nonvanishing. Prove these assertions. For $n := 0$ this is just Newton's method, for $n := 1$ it is Halley's method. (See Householder [70].)

b) Let

$$x_{k+1} := x_k(1 + (1 - yx_k) + (1 - yx_k)^2) .$$

Show that

$$\left(x_{k+1} - \frac{1}{y}\right) = y^2\left(x_k - \frac{1}{y}\right)^3$$

and that for x_0 sufficiently close to $1/y$, x_k converges cubically to $1/y$.

c) Let

$$x_{k+1} := \tfrac{1}{8}x_k(15 - 10x_k^2 y + 3y^2 x_k^4) .$$

Show that

$$yx_{k+1}^2 - 1 = \tfrac{1}{64}(9y^2x_k^4 - 33yx_k^2 + 64)(yx_k^2 - 1)^3$$

and that for x_0 sufficiently close to $1/\sqrt{y}$, x_k converges cubically to $1/\sqrt{y}$.

d) Show that b) and c) require fewer multiplications than (6.4.3) or (6.4.6) for computation of reciprocals and square roots. These are, in practice, very good high precision algorithms.

4. Let $x_0 := 1$ and let

$$x_{k+1} := 2x_k - x_k^2 x$$

be the iteration (6.4.3) for computing $1/x$. Show that x_{k+1} is the $(2^{k+1} - 1)$th Taylor polynomial of $f(x) := 1/x$ expanded around the point 1. Thus for division we may think of Newton's method as a means of accelerating the computation of the Taylor series.

5. Let $x_0 := 1$ and let

$$x_{k+1} := \frac{1}{2}\left(x_k + \frac{x}{x_k}\right)$$

be the iteration (6.4.6) for computing $\sqrt{x}$. Show that x_{k+1} is a rational function $r(x)$ with numerator of degree 2^k and denominator of degree $2^k - 1$ that satisfies

$$|\sqrt{x} - r(x)| = O(x-1)^{2^{k+1}} .$$

[This implies that $r(x)$ is the $(2^k, 2^k - 1)$ Padé approximant to $\sqrt{x}$ at 1. See Section 10.1.]

6. Invert $1/x^2 - y$ to calculate $\sqrt{y}$ without using any divisions.

7. (*Other equivalences*; *Brent* [76c])

a) Show that squaring is equivalent to multiplication by considering $(a+b)^2 - (a-b)^2$.

b) Complete the proof of Theorem 6.3 by showing that square root extraction is equivalent to multiplication.
Hint:

$$(1 + 2\delta x)^{1/2} = 1 + \delta x - \frac{\delta^2}{2}x^2 + O((\delta x)^3) .$$

Use $\delta := 10^{-m}$ for appropriate m to reduce the computation of x^2 to root extraction and $O_B(n)$ operations.

c) Show that inversion is equivalent to multiplication.
d) Show that pth-root extraction is equivalent to multiplication.

8. a) Suppose that $C_f(n)$ is the bit complexity of calculating n digits of f. Assume that $C_f(n)$ is increasing and that $C_f(2n) \geq 2C_f(n)$. Suppose that f satisfies the conditions of Corollary 6.1. Show that $\dot{f}$ has at worst the same bit complexity as f, and that

$$C_{f^{-1}}(n) = O_B(C_f(n) + M(n)) .$$

b) Write down Newton's method for computing exp from log and log from exp. These particularly simple iterations combine with a) to show that the problems of calculating exp and log are effectively equivalent, from a bit complexity viewpoint.

9. (*Fast base conversion*; *Schönage*) Let k and j be fixed integers. Show that an n-"digit" base k number can be converted into base j with bit complexity

$$O_B(\log n\, M(n)) .$$

Hint: Break the number to be converted in half (base k), convert each half, and recombine. (See Knuth [81] for a lengthy discussion of this problem.)

10. a) Show that $n!$ can be calculated with bit complexity

$$O_B(\log n\, M(n \log n)) .$$

Hint: First calculate $1 \times 2, 3 \times 4, \ldots$. Then calculate $1 \times 2 \times 3 \times 4$, $5 \times 6 \times 7 \times 8, \ldots$ etc.

b) Compare this to calculating $n!$ as in Exercise 3 of Section 6.1. Show that no multiplication can reduce this method below $O(n^2)$. [The best known bound for $n!$ is $O_B((\log\log n)M(n \log n))$; see P. B. Borwein [85].]

Chapter Seven

Algorithms for the Elementary Functions

Abstract. *We analyze algorithms for the transcendental elementary functions based on the transformation theory for elliptic integrals and in particular on the AGM.*

7.1 π AND LOG

All the elementary transcendental functions can be calculated with bit complexity $O_B(\log n\, M(n))$. This is a consequence of the fact that log has operational complexity $O_{\mathrm{op}}(\log n)$, and hence has bit complexity $O_B(\log n\, M(n))$. The approach to log rests most easily on the logarithmic asymptotic of K at 1. Before proceeding with this analysis it is convenient to record the complexity of the algorithms for π, based either on iterating the modular equation, W_p, or more specially on the AGM.

Theorem 7.1

The initial n digits of π can be calculated with operational complexity

$$O_{\mathrm{op}}(\log n)$$

and with bit complexity

$$O_B(\log n\, M(n)) .$$

Proof. Both Algorithms 2.1 and 2.2 as well as most of those of Chapter 5 perform with the above complexity. □

In all of the above algorithms some of the calculation may be done to reduced precision. For example, in Algorithm 2.1 the computation of x_n and y_n, which both tend to 1 quadratically, can be performed at successively lower precision. The saving, however, is only in the constant term, reducing it by a factor of less than 2.

We record the following estimates:

Theorem 7.2

(7.1.1) $$\left|K'(k) - \log\left(\frac{4}{k}\right)\right| = O(|k^2 \log k|) \qquad \mathrm{re}(k) > 0$$

(7.1.2) $$|E'(k) - 1| = O(|k^2 \log k|) \qquad \mathrm{re}(k) > 0$$

(7.1.3) $$\left|K'(k) - \log\left(\frac{4}{k}\right)\right| \leq 10|k^2 \log k| \qquad k \in (0, 10^{-3})$$

(7.1.4) $$|E'(k) - 1| \leq 10|k^2 \log k| \qquad k \in (0, 10^{-3}).$$

Proof. The relationships for K are in Exercise 4 of Section 1.3. (See also Exercise 1 of Section 2.3.) For (7.1.2) observe that by (1.3.2), for $0 < k < 1$

$$E'(k) - 1 = \int_0^1 \frac{\sqrt{1-(1-k^2)t^2} - \sqrt{1-t^2}\, dt}{\sqrt{1-t^2}}$$

$$\leq \int_0^1 \frac{k^2 t^2\, dt}{\sqrt{[1-(1-k^2)t^2](1-t^2)}} \leq k^2 K'(k).$$

The constant in (7.1.4) requires a little additional scrutiny. □

The following approach to calculating log is essentially due to Salamin (in Beeler et al. [72]).

Algorithm 7.1

For $x \in (\frac{1}{2}, 1)$ and $n \geq 3$,

(7.1.5) $$|\log x - K'(10^{-n}) + K'(10^{-n}x)| \leq \frac{n}{10^{2(n-1)}}$$

where

$$K'(10^{-n}) = \frac{\pi}{2\mathrm{AG}(1, 10^{-n})}$$

and

$$K'(10^{-n}x) = \frac{\pi}{2\mathrm{AG}(1, 10^{-n}x)}$$

are computed from the AGM iteration.

This algorithm has operational complexity $O_{\mathrm{op}}(\log n)$ and bit complexity $O_B(M(n) \log n)$.

Proof. The estimate (7.1.5) is immediate from Theorem 7.2. The computation of the two elliptic integrals requires precomputing π, which has complexity $O_{\mathrm{op}}(\log n)$. The final detail is that $\mathrm{AG}(1, 10^{-n}x)$ and $\mathrm{AG}(1, 10^{-n})$ can be calculated to precision $2n$ using $O(\log n)$ iterations of the AGM iteration. (See Exercise 1.) □

A related algorithm that avoids precomputing π can be established from Algorithm 1.2 (which provides a direct calculation of K'/E').

Algorithm 7.2

Let $R'(k) := K'(k)/E'(k)$. For $x \in (\frac{1}{2}, 1)$ and $n \geq 3$,

(7.1.6) $$|\log x - R'(10^{-n}) + R'(10^{-n}x)| \leq \frac{n}{10^{2(n-2)}}$$

where

(7.1.7) $$R'(k) = \frac{1}{1 - \sum_{n=0}^{\infty} 2^{n-1} c_n^2}$$

and c_n is associated with the AGM process commencing with $a_0 := 1$ and $b_0 := k$. [See equation (1.1.3).]

This algorithm has operational complexity $O_{\mathrm{op}}(\log n)$ and bit complexity $O_B(M(n) \log n)$.

The proof is straightforward and is left as an exercise. Both of the above algorithms are based on an underlying quadratic method for calculating K' and E'. Algorithms based on pth-order methods can be constructed as in Chapter 5. A quartic version, for example, can be derived from Exercise 3 of Section 1.4. Instead of calculating R' from the AGM, we use

(7.1.8) $$R'(k) = \frac{1}{1 - \sum_{n=0}^{\infty} 4^n[\alpha_n^4 - [(\alpha_n^2 + \beta_n^2)/2]^2]}$$

where

$$\alpha_{n+1} := \frac{\alpha_n + \beta_n}{2} \quad \text{and} \quad \beta_{n+1} := \left(\frac{\alpha_n^3\beta_n + \beta_n^3\alpha_n}{2}\right)^{1/4}$$

and

$$\alpha_0 := 1 \quad \text{and} \quad \beta_0 := k^{1/2}.$$

In this, as in other quartic versions of quadratic algorithms, there is a substantial computational saving (as much as 35%).

Comments and Exercises

The algorithms of this section for log all suffer from the drawback that they are not truly iterative. Increasing the precision requires choosing new starting values. This is more of an aesthetic than a computational problem; even with iterative methods one only computes to a fixed precision, and increasing the accuracy usually entails starting at least one of the calculations all over again. While two different AGM or related processes must be calculated for the initial value of log, subsequent values require computing only a single AGM since one of the terms can be reused. These methods are quite stable, requiring only $O(\log\log n)$-guard digits. They will outcompete traditional methods—depending enormously on implementation—in the several-hundred-digit range.

The algorithms of this section are the asymptotically fastest known algorithms for log (see Section 10.2) and are faster than any known algorithms based on other methods, although $O_B((\log n)^2 M(n))$ can be achieved by techniques of Chapter 10. These types of algorithms were first examined by Salamin (Beeler et al. [72]) and independently by Brent [76*a*, *b*, and *c*]. Newman [82] gives a self-contained account, as do Borwein and Borwein [84*a*]. The second algorithm is in Borwein and Borwein [84*d*].

Finally, while we have only presented the algorithms for real k, they extend naturally into the complex plane; only the error estimates become slightly more complicated. (See Exercise 1.) Matrix versions due to Stickel [85] are discussed in Exercise 6.

1. Show that Algorithm 7.1 can be used to calculate log uniformly for $\{z \in \mathbb{C} \mid |z-1| < \frac{1}{2}\}$ with operational complexity $O_{\mathrm{op}}(\log n)$ and bit complexity $O_B(\log n\, M(n))$.
2. Examine the convergence of the AGM for $a_0 := 1$ and $b_0 := 10^{-n}$. Specifically, estimate the number of iterations required to produce an answer within 10^{-n} of the limit. For Algorithms 7.1 and 7.2, find a reasonable bound on the number of iterations of the AGM required to produce a 1000-digit precision algorithm for $\log x$, $x \in (\frac{1}{2}, 1)$.
3. (*An asymptotic algorithm for* π) Show that, for $n \ge 3$,

$$\left|\log(1+10^{-n}) - \frac{\pi}{2}\left[\frac{1}{\mathrm{AG}(1,10^{-n})} - \frac{1}{\mathrm{AG}(1,10^{-n}+10^{-2n})}\right]\right| \le n10^{2-2n},$$

and hence

$$\left|\frac{2}{\pi} - \left[\frac{10^n}{\mathrm{AG}(1,10^{-n})} - \frac{10^n}{\mathrm{AG}(1,10^{-n}+10^{-2n})}\right]\right| \le n10^{2-n}.$$

This provides an $O_{\mathrm{op}}(\log n)$ algorithm for π. (See Newman [82] or Borwein and Borwein [84*a*].)

4. Given the pth-order modular equation Ω_p (as in Section 4.5), show how to construct asymptotic algorithms for log analogous to Algorithms 7.1 and 7.2, but with an underlying pth-order iteration.
5. Show how the series expansion for K' and E' of Section 1.3 can be combined with Algorithms 7.1 and 7.2 to provide $O_{\mathrm{op}}(\log n)$ algorithms for log that provide n digits of log using starting values $10^{-n/k}x$ and $10^{-n/k}$.
6. (*The matrix AGM*) Let $\mathcal{P}_N$ denote the $N \times N$ self-adjoint positive definite matrices and let I denote the $N \times N$ identity matrix. Let $A_0 := A \in \mathcal{P}_N$, $B_0 := I$,

$$\text{(7.1.9}i\text{)} \qquad A_{n+1} := \tfrac{1}{2}(A_n + B_n)$$

$$\text{(7.1.9}ii\text{)} \qquad B_{n+1} := \sqrt{A_n B_n}.$$

   a) Show that if $A \in \mathcal{P}_N$, then there exists a unique $C \in \mathcal{P}_N$ so that $C^2 = A$. *Hint*: The iteration $C_{n+1} := C_n + \frac{1}{2}(A - C_n^2)$, $C_0 := 0$ converges to C.
   b) Suppose that $X_0 \in \mathcal{P}_N$ commutes with $A \in \mathcal{P}_N$. Show that, for X_0 sufficiently close to $\sqrt{A}$, Newton's method $X_{n+1} := \frac{1}{2}(X_n + AX_n^{-1})$ converges to $\sqrt{A} \in \mathcal{P}_N$ quadratically.
   c) Show that the matrix AGM (7.1.9) converges to a matrix $\mathrm{AG}(A, I) \in \mathcal{P}_N$ and show that $A_n - B_n$ converges quadratically to zero.
   d) Show that

$$\frac{\pi}{2}\mathrm{AG}(A,B)^{-1} = \int_{-\infty}^{\infty} [(x^2I + A^2)(x^2I + B^2)]^{-1/2}\,dx.$$

   Hint: Imitate the second proof of Theorem 1.1 and use the fact that A_n and B_n commute.
   e) Let

$$K(A) := \int_0^{\pi/2} \frac{d\theta}{\sqrt{I - A^2\sin^2\theta}}$$

   and let $K'(A) = K(\sqrt{I - A^2})$. Suppose that $A \in \mathcal{P}_N$ and also that $0 < a \le \|A\|_\infty \le b$. Show for large n that (7.1.5) holds, namely, there exists c so that

$$\text{(7.1.10)} \qquad \|\log A - K'(10^{-n}I) + K'(10^{-n}A)\|_\infty \le \frac{cn}{10^{2n}}.$$

f) Show that this provides an $O_{op}(\log n)$ algorithm for the matrix logarithm of $A \in \mathcal{P}_N$ and, by inversion, an $O_{op}((\log n)^2)$ iteration for the matrix exponential.

For further details, and extensions beyond the positive definite case see Stickel [85], where computational experience is also indicated.

7.2 *THETA FUNCTION ALGORITHMS FOR LOG*

We start with the fundamental identity of Chapter 2

$$\pi \frac{K(k')}{K(k)} = \log\left(\frac{1}{q}\right) \tag{7.2.1}$$

and the series expansion

$$\frac{K(k)}{\pi} = \frac{1}{2}\left(\sum_{-\infty}^{\infty} q^{n^2}\right)^2 = \frac{1}{2}\,\theta_3^2(q)\,. \tag{7.2.2}$$

We recall that

$$k = \frac{\theta_2^2(q)}{\theta_3^2(q)} = \left[\frac{\Sigma_{-\infty}^{\infty} q^{(n+1/2)^2}}{\Sigma_{-\infty}^{\infty} q^{n^2}}\right]^2. \tag{7.2.3}$$

The algorithm for $\log(1/q)$ is now:

Algorithm 7.3

Fix $q \in (a, b)$ with $0 < a < b < 1$.
Step 1: Calculate $K(k)/\pi$ from (7.2.2).
Step 2: Calculate k from (7.2.3).
Step 3: Calculate $K(k')$ using the AGM commencing with 1 and k.
Step 4: Calculate $\log(1/q) = \pi[K(k')/K(k)]$.

This algorithm has operational complexity $O_{op}(\sqrt{n})$ and bit complexity $O_B(\sqrt{n}\, M(n))$.

The algorithm's complexity is determined by the series expansions employed in steps 1 and 2. These "sparse" series yield n-digit accuracy after $\sqrt{n}$ nonzero terms. While the asymptotic complexity is far from optimal, the algorithm has the advantage of not requiring very small starting values for the AGM iteration (Step 3). Also, only a single AGM iteration is required. Sasaki and Kanada [82], who proposed and analyzed the above algorithm, show that it out performs the methods of Section 7.1 for numbers in the 3000-digit range. Note that π must be precomputed. As Sasaki and Kanada observe, the algorithm may be accelerated by using

$$m \log\left(\frac{1}{q}\right) = \log\left(\frac{1}{q^m}\right) \tag{7.2.4}$$

for various m. This speeds up the series calculation at the expense of the AGM. For n-digit precision, using $m = n$ effectively reduces this algorithm to Algorithm 7.1. (See Exercise 1.)

For certain choices of q we get reduction in complexity. If q is any small integer, then the series expansions are particularly easy to evaluate. (See Exercise 2.) This leads to a very fast algorithm for $\pi/\log 10$ (using base 10 arithmetic) as follows. From (7.2.1), (7.2.2), and (7.2.3) we have

$$\log\left(\frac{1}{q}\right) = \pi \frac{K'}{K}(k) = \theta_3^2(q) M(1, k) = \frac{\pi}{\mathrm{AG}(\theta_3^2(q), \theta_2^2(q))} \tag{7.2.5}$$

or

$$\frac{\pi}{\log(1/q)} = \mathrm{AG}\left(\left(\sum_{-\infty}^{\infty} q^{n^2}\right)^2, \left(\sum_{-\infty}^{\infty} q^{(n+1/2)^2}\right)^2\right). \tag{7.2.6}$$

Now for $q := 1/10^4$ both of the above series are just sequences of 0's and 1's and the starting values for the mean iteration can be calculated very quickly $[O_B(M(n))]$. The remainder of the work involves calculating a single AGM. Similarly $\pi/\log p$ is amenable to very fast computation in base p.

Properly interpreted, (7.2.6) remains valid for matrices and provides a theta-based computation of the matrix logarithm of a positive definite matrix. (See Exercise 3.)

Comments and Exercises

Further discussion of material in this section may be found in Sasaki and Kanada [82] and in Borwein and Borwein [84*d*]. Sasaki and Kanada compare Algorithm 7.3 to algorithms for log based on Taylor series for $\log(1 + x)$ and $\log[(1 + x)/(1 - x)]$ and conclude that for more than (roughly) 100 decimal digits the Taylor series methods are slower.

1. Show that (7.2.4) for various m can be combined with Algorithm 7.3 to provide algorithms for log of any complexity between $O_{op}(\sqrt{n})$ and $O_{op}(\log n)$.

2. Discuss the bit complexity of calculating $\theta_2(q)$, $\theta_3(q)$, and $\theta_4(q)$, where q is the reciprocal of a fixed integer. Show, for p integral, that (7.2.6) can be used to calculate $\pi/\log p$ with bit complexity $O_B(\log n\, M(n))$. (See Exercise 9 of Section 6.4.)

3. Consider the matrix AGM of Exercise 6 of the previous section. Establish a matrix version of (7.2.1) to (7.2.6). Then construct an algorithm for the matrix log based on (7.2.6).

7.3 *THE COMPLEXITY OF ELEMENTARY AND ELLIPTIC FUNCTIONS*

The algorithms of Section 7.1 can be inverted by Newton's method to provide algorithms for exp with bit complexity $O_B(\log n\, M(n))$ and operational complexity $O_{\text{op}}((\log n)^2)$. From a bit complexity point of view, this is the best known bound. Since we can invert log in $\{|z-1| \le \frac{1}{2}\}$, we can produce an algorithm for exp in a complex neighbourhood of zero and hence have $O_B(\log n\, M(n))$ algorithms for all the trigonometric functions. Exercises 1 and 2 give some variations. In fact, for any elementary function we have the following:

***Theorem* 7.3**

Any elementary function f over $\mathbb{Q}(x)$ can be calculated uniformly (in bounded regions where f is single valued and analytic) with bit complexity

$$O_B(\log n\, M(n))$$

and with operational complexity

$$O_{\text{op}}((\log n)^s)$$

where s is a constant depending only on f.

Proof. For our purposes the elementary functions are the rational functions, log and exp, and any function that can be formed from these functions by a finite number of compositions, multiplications, additions, and solutions of algebraic equations. (See Davenport [81] or Ritt [48].) The point of the proof is that such an f is constructed from $\mathbb{Q}(x)$ by taking a finite number of exponentials, logarithms, and solutions of algebraic equations in these quantities. The number of algebraic equations to be solved determines the constant s. As in Chapter 6, solution of the algebraic equation in question can be effected in a time proportional to the complexity of evaluating the equation. □

A number of comments are in order. First, we can formulate the above theorem for f algebraic over $\mathbb{R}(x)$ if we assume that the requisite real numbers are given. Second, while multiple solutions of an algebraic equation pose no theoretical problem, in practice, determining the "correct root" can be a major nuisance. For a multiple-valued function the theorem must be interpreted as guaranteeing some value of the function. This is inevitable. It is not even clear what it should mean to compute an infinite-valued function.

That the operational complexity behaves like $(\log n)^s$ instead of $(\log n)$ reflects in part that operational complexity is an inappropriate measure when Newton's method is involved. While the preceding algorithms for log require most of the operations to be done to full precision, this is no longer the case for this approach to other transcendental elementary functions.

Since we can calculate elliptic integrals with bit complexity $O_B(\log n\, M(n))$ (Exercise 5 of Section 1.4 and Exercise 2 of this section), we can calculate the Jacobian elliptic functions with similar dispatch.

It is not clear which other nonelementary transcendental functions have bit complexity $O_B(\log n\, M(n))$. Does, for example, the gamma function? Nor is it clear whether the bit complexity $O_B(\log n\, M(n))$ is best possible for the nonalgebraic elementary functions. The best known lower bound for log and exp is the virtually trivial bound of $O_B(M(n))$. (See Exercise 3.)

Comments and Exercises

The algorithms for exp (see also Exercises 1 and 2) require inversion and are much less satisfactory than the algorithms for log. A direct $O_B((\log n)^2 M(n))$ algorithm is presented in Chapter 10. There are a number of issues that remain unresolved in this discussion. The most obvious is a discussion of lower bounds. Observe that, by Theorem 6.4, showing that exp does not have complexity $O_B(M(n))$ would show that exp is a transcendental function. Likewise, showing that π does not have bit complexity $O_B(M(n))$ would imply the transcendence of π. The gap between the known operational complexities for log $[O_{\text{op}}(\log n)]$ and exp $[O_{\text{op}}((\log n)^2)]$ is probably specious, but this also is not known. We will show in Section 8.8 that direct algorithms for exp and log of the type that we derived for K in Chapter 1 cannot exist. There are no quadratically convergent fixed iterations for these functions.

1. From (2.3.7) and Exercise 3 of Section 2.5,

$$\lim_{n\to\infty}\left(\frac{4a_n}{c_n}\right)^{2^{-n}} = \exp\left[\frac{\pi}{2}\lim_{n\to\infty}\left(\frac{a_n}{a_n^*}\right)\right]$$

where a_n and c_n are generated from the AGM commencing with $a_0 := 1$ and $b_0 := k'$, while a_n^* is generated from the AGM commencing with $a_0^* := 1$ and $b_0^* := k$. Show that this leads to an $O_B(\log n\, M(n))$ algorithm for e^x, which begins by solving for $a_n/a_n^* = \pi x/2$.

2. (*A more direct approach to tan*) As in Exercise 5 of Section 1.4 and Theorem 2.6 of Section 2.6, we have the Landen transform for

$$F(\phi, k) := \int_0^\phi \frac{d\theta}{\sqrt{1-k^2\sin^2\theta}} \qquad k \in [0,1), \quad \phi \geq 0 .$$

If

$$k_{n+1} := \frac{1-k_n'}{1+k_n'} \qquad \text{and} \qquad \tan(\phi_{n+1}-\phi_n) = k_n' \tan \phi_n$$

then, as before,

$$F(\phi_{n+1}, k_{n+1}) = (1+k_n')F(\phi_n, k_n) \tag{7.3.1}$$

and

$$F(\phi_0, k_0) = \left[\prod_{n=0}^{\infty}\left(\frac{2}{1+k_n'}\right)\right] \lim_{n\to\infty} \frac{\phi_n}{2^n} . \tag{7.3.2}$$

a) Show that

$$F(\phi_0, k) = \phi_0 + O(k^2) \qquad \text{as} \qquad k \to 0 .$$

b) Show that

$$F(\phi_0, k) = \log\tan\left(\frac{\pi}{4}+\frac{\phi_0}{2}\right) + O(1-k) \qquad \text{as} \qquad k \to 1 .$$

c) Show that if $w_n := \tan\phi_n$, then

$$w_{n+1} = \frac{(1+k_n')w_n}{1-k_n' w_n^2} .$$

d) Thus

$$\begin{aligned}\phi_n &= F(\phi_n, k_n) + O(k_n^2)\\ &= \left[\prod_{m=0}^{n-1}\left(\frac{1+k_m'}{2}\right)\right]\log\tan\left(\frac{\pi}{4}+\frac{\phi_0}{2}\right) + O(k_n^2 + (1-k_0))\end{aligned}$$

or

$$\begin{aligned}\tan^{-1} w_n &= \left[\prod_{m=0}^{n-1}\left(\frac{1+k_m'}{2}\right)\right]\log\tan\left(\frac{\pi}{4}+\frac{\tan^{-1} w_0}{2}\right)\\ &\quad + O(k_n^2 + (1-k_0))\\ &= \left[\prod_{m=0}^{n-1}\left(\frac{1+k_m'}{2}\right)\right]\log\delta + O(k_n^2 + (1-k_0))\end{aligned}$$

where $\delta := \sqrt{w_0^2+1} + w_0$. Show, by inverting c), that $\tan^{-1}$ can be calculated from log with complexity $O_B(\log n\, M(n))$. Show that, by inverting the above, tan can be calculated from log with complexity $O_B(\log n\, M(n))$.

This approach, which avoids using complex arithmetic to access the trigonometric functions, is essentially due to Brent [76*a*].

3. Let $L(n)$ denote the bit complexity for evaluating n digits of log. Show that

$$D(n) = O_B(L(n))$$

and hence, log and exp are at least as complex as multiplication. *Hint*: Consider computing the derivative of log.

Chapter Eight

General Means and Iterations

Abstract. *In Section 8.1 we define abstract means and discuss their behavior. In Section 8.2 we discuss equivalent means. In the next three sections we consider general mean iterations and examine their convergence properties. Later sections concern Taylor expansions of means, multidimensional means, and related questions. The final section considers algebraic mean iterations and the possibility of extracting elementary limits from such iterations.*

8.1 ABSTRACT MEANS

There is a large literature on means but little agreement as to what exactly constitutes a mean. For our purposes we have

Definition 8.1

(*a*) A *mean* is a continuous real-valued function M of two strictly positive real variables a and b such that

(8.1.1) $$a \wedge b \le M(a, b) \le a \vee b$$

for all $a>0$ and $b>0$. We denote $a \wedge b := \min(a, b)$ and $a \vee b := \max(a, b)$. (Continuity is not always essential. On occasion we will refer to possibly discontinuous functions satisfying the above definition as *discontinuous means*.)

(*b*) A mean is *strict* if, in addition, it is *diagonal*:

(8.1.2) $$M(a, b) = a \quad \text{or} \quad M(a, b) = b$$

if and only if $a = b$.

(*c*) A mean is *homogeneous* if

(8.1.3) $$M(\lambda a, \lambda b) = \lambda M(a, b)$$

for $a, b, \lambda > 0$.

(*d*) A mean is *symmetric* if

(8.1.4) $$M(a, b) = M(b, a)$$

for $a, b > 0$.

(*e*) A mean is (strictly) *isotone* if, for $a, b > 0$,

(8.1.5) $$M(a, \cdot) \quad \text{and} \quad M(\cdot, b) \quad \text{are (strictly) increasing}.$$

We will find it convenient to consider the *trace* t_M of a mean M given by $t_M(x) := M(x, 1)$. We gather up some useful properties of means whose proofs are left as Exercise 1.

Proposition 8.1

(*a*) Every diagonal continuous (strictly), isotone mapping is a (strict) mean.

(*b*) Suppose that M is symmetric and homogeneous. Then M is isotone if and only if its trace t_M is isotone.

(*c*) The isotone, (symmetric), (strict), (homogeneous) means form a convex set.

(*d*) The symmetric, (homogeneous) means form a uniformly closed convex set.

(*e*) Let M and N be (strict) means. Then any continuous mapping P such that

$$M(a, b) \ge P(a, b) \ge N(a, b) \qquad a, b > 0$$

is a (strict) mean.

Corresponding to each mean M we associate another mean M_p, defined by

(8.1.6) $$M_p(a, b) := [M(a^p, b^p)]^{1/p} \qquad p \ne 0.$$

Then $M = (M_{-1})_{-1}$ and M_{-1} is strict, symmetric, homogeneous, or isotone whenever M is, and $t_{M_{-1}}(x) = t_M^{-1}(1/x)$. This is a special way of building an *equivalent* mean as we now discuss.

For any strictly monotone (increasing or decreasing) function $f: \mathbb{R}^+ \to \mathbb{R}^+$ we define the mean

$$M_f(a, b) := f^{-1}(M(f(a), f(b))).$$

When $f(x) := x^p$ (we write $f := \iota^p$) we denote M_f by M_p [consistently with (8.1.6)]. It is easy to check that M_f is a strict, symmetric, or isotone mean whenever M is. (See Exercise 2.) To give our discussion some flesh, we introduce four of the most useful classes of means. In this chapter we reserve the letters M and N for general means.

The Holder Means

For $p \in \mathbb{R}^\times$ let

$$(8.1.7) \qquad H_p(a,b) := \left(\frac{a^p + b^p}{2}\right)^{1/p} \qquad a, b > 0\,.$$

Then H_1 is just the arithmetic mean A, and thus H_p is a strict, homogeneous, symmetric, isotone mean. Moreover, $\lim_{p\to 0} H_p(a,b) = \sqrt{ab}$ is the geometric mean G and may reasonably be denoted by H_0. (See Exercise 14.) Since $H_{-1} \le H_0 \le H_1$, Proposition 8.1(*e*) shows H_0 to be a strict mean. For all p one can unambiguously define H_p for $a, b \ge 0$. Then the trace of H_p satisfies

$$(8.1.8) \qquad t_{H_p}(\mathbb{R}^+) = \begin{cases} [2^{-1/p}, \infty) & p \ge 0 \\ [0, 2^{-1/p}) & p < 0 \end{cases}.$$

Note also that $(H_p)_{-1} = H_{-p}$ and that $H_p = A_p$.

Another useful way of building means is based on the next proposition.

Proposition 8.2

Let M be an isotone, homogeneous mean. Then, for $p \in \mathbb{R}$,

$$(8.1.9) \qquad {}_pM(a,b) := \frac{M(a^p, b^p)}{M(a^{p-1}, b^{p-1})} = \frac{M_p^p(a,b)}{M_{p-1}^{p-1}(a,b)}$$

defines another homogeneous mean, ${}_pM$, which is strict or symmetric whenever M is strictly isotone or symmetric.

Proof. This is left as Exercise 4a). □

The Lehmer Means

For $p \in \mathbb{R}$ we let

$$(8.1.10) \qquad L_p(a,b) := \frac{a^p + b^p}{a^{p-1} + b^{p-1}}\,.$$

Since $L_p = {}_p(H_1)$, each L_p is a symmetric, homogeneous, strict mean. Since $t_{L_p}(x) = (x^p + 1)/(x^{p-1} + 1)$, L_p is isotone only for $0 \le p \le 1$. Moreover, $L_1 = H_1$, $L_{1/2} = H_0$, $L_0 = H_{-1}$, and (by Exercise 5 of Section 8.6) these are

the only means common to the Lehmer and Holder classes. Again there is no difficulty extending L_p to $a, b \ge 0$ and

$$(8.1.11) \qquad t_{L_p}(0) = \begin{cases} 1 & p > 1 \\ \frac{1}{2} & p = 1 \\ 0 & p < 1 \end{cases} \quad \text{and} \quad t_{L_p}(\infty) = \begin{cases} \infty & p > 0 \\ 2 & p = 0 \\ 1 & p < 0 \end{cases}$$

where, here and below, we write $f(\infty)$ for $\lim_{x\to\infty} f(x)$. To see this, use

$$(8.1.12) \qquad (L_p)_{-1}(a,b) = \frac{ab^p + ba^p}{a^p + b^p} = {}_{(1-p)}(L_1)(a,b) = L_{(1-p)}(a,b).$$

Indeed, generally

$$(8.1.13) \qquad ({}_pM)_{-1} = {}_{(1-p)}M\,.$$

The Gini Means

Let r and s be given. Consider $f = \iota^q$ where $q := s - r$. Then

$$(8.1.14) \qquad f^{-1}L_{s/(s-r)}(f(a), f(b)) = \left[\frac{a^s + b^s}{a^r + b^r}\right]^{1/(s-r)} =: G_{s,r}(a,b)$$

defines the Gini mean $G_{s,r}(a,b)$. (See Gini [38].) Moreover (8.1.14) shows that $G_{s,r}$ is indeed a strict, homogeneous mean.

Proposition 8.3

Let f be a continuous strictly monotone function of a nonnegative variable. Then

$$(8.1.15) \qquad M_{\int f}(a,b) := f^{-1}\left[\frac{\int_a^b f(x)\,dx}{b-a}\right] \qquad a \ne b$$

extends to a symmetric, (generally nonhomogeneous), strict, continuous mean.

Proof. The integral mean value theorem gives the conclusion, bar the continuity. This follows from the continuity of the definite integral. □

We immediately apply this to Stolarsky's power means (Stolarsky [75, 80]).

Stolarsky's Means

Let $p \in \mathbb{R}$ and denote $M_{\int \iota^{p-1}}$ by S_p. Then S_p is a homogeneous, symmetric, strict mean given by

$$(8.1.16i) \qquad S_p(a,b) = \left[\frac{a^p - b^p}{p(a-b)}\right]^{1/(p-1)} \qquad p \neq 0, 1$$

with

$$(8.1.16ii) \qquad S_0(a,b) = \lim_{p\to 0} S_p(a,b) = \frac{b-a}{\log b - \log a} =: \mathcal{L}(a,b)$$

and

$$(8.1.16iii) \quad S_1(a,b) = \lim_{p\to 1} S_p(a,b) = e^{-1}(a^a b^{-b})^{1/(a-b)} =: \mathcal{I}(a,b)\,.$$

The mean $\mathcal{L}$ is the *logarithmic mean* and $\mathcal{I}$ is the *identric mean*. These means have

$$t_{S_p}(0) = \begin{cases} p^{-1/(p-1)} & p>0,\ p\neq 1 \\ e^{-1} & p=1 \\ 0 & p\leq 0 \end{cases} \qquad \text{and} \qquad t_{S_p}(\infty) = \infty\,.$$

Also

$$\frac{\dot{t}_{S_p}(x)}{t_{S_p}(x)} = \frac{1}{(p-1)}\,\frac{(p-1)x^p - px^{p-1}+1}{(x^p-1)(x-1)}$$

so that $S_p(a,b)$ is increasing in (a,b) for all p in $\mathbb{R}$. This, in part, follows from the inequality $(1-p)x^p + px^{p-1} \geq 1$ for $0 \leq p \leq 1$.

All of the means in these classes are *piecewise monotone* in the sense that $\dot{t}_M(x)$ has only finitely many sign changes. Thus there is no difficulty in defining $M(0,b) = bM(0,1) = b\lim_{x\downarrow 0} t_M(x)$ in all these homogeneous cases, and we can freely consider M defined on $\mathbb{R}^{+2} := \{(x,y) | x \geq 0,\ y \geq 0\}$ and at ∞. We will do so from now on. Note also that when M is continuous, $t_M([0,\infty]) = [0,\infty]$ is equivalent to $t_M(0) = 0$ and $t_M(\infty) = \infty$.

An elementary but very useful proposition is next. The proof is left for Exercise 11.

Proposition 8.4 **(*Composition*)**

If M is defined by

$$M(a,b) := M_0(M_1(a,b), M_2(a,b))$$

where M_i, $i = 0, 1, 2$, are means, then M is a mean. If two of M_0, M_1, M_2 are strict, so is M. If all three are homogeneous, symmetric, or isotone, then so is M.

For example, $M \vee N$ and $M \wedge N$ are strict means whenever M and N are. So is any mean *between* them, in the sense of Proposition 8.1 (*e*).

There are many highly pathological means, as Exercise 12 shows. This is particularly so in the absence of continuity. For future reference we will say that a homogeneous mean is *ultimately monotone* if $M(x,1)$ and $M(1,x)$ are monotone in some neighbourhood of zero and ∞. We write $M \leq N$ if $M(a,b) \leq N(a,b)$ for all $a, b > 0$.

Comments and Exercises

There is a great literature on particular means and very little on means in general. Much classical information can be found in Hardy, Littlewood, and Polya [59] and in the other references scattered throughout the chapter.

1. Prove Proposition 8.1.

2. Establish that for any mean M and any strictly monotone $f: \mathbb{R}^+ \to \mathbb{R}^+$, $M_f(a,b) := f^{-1}M(f(a), f(b))$ defines a mean which is strict, symmetric, or isotone whenever M is. Moreover, if f is ι^p, $p \in \mathbb{R}^\times$, then M_f is homogeneous whenever M is.

3. a) Show that $H_p(a,b)$ is a continuous increasing function of p with $\lim_{p\to\infty} H_p = \vee$ and $\lim_{p\to-\infty} H_p = \wedge$.
b) Establish the assertions about the Holder means.
c) If M is homogeneous and symmetric, then $M_0 = G$, whenever M_0 exists as a limit.

4. a) Prove Proposition 8.2.
b) Establish the assertions about the Lehmer means.

5. (*Isotonicity of* $\mathrm{M_p}$) Let $\Phi(a) := a\log a$ for $a > 0$, and let M be a differentiable mean.

a) Show that $M_p(a,b)$ is isotone in $p > 0$ if and only if

$$(8.1.17) \qquad \Phi(a)\,\frac{\partial M(a,b)}{\partial a} + \Phi(b)\,\frac{\partial M(a,b)}{\partial b} \geq \Phi(M(a,b))\,.$$

b) Suppose that M is also homogeneous. Then

$$a\,\frac{\partial M(a,b)}{\partial a} + b\,\frac{\partial M(a,b)}{\partial b} = M(a,b)\,.$$

c) Use a), b), and the convexity of Φ to show that H_p is increasing for p in $\mathbb{R}$.
d) If M is homogeneous and symmetric and if M_p is increasing for $p > 0$, then M_p is increasing for p in $\mathbb{R}$, whenever M_0 exists.

6. Suppose M_p is isotone in p. Then

i) ${}_pM \geq M_p \qquad p \geq 1$
ii) ${}_pM \leq M_p \qquad p \leq 1$
iii) ${}_pM \leq M_{p-1} \qquad p \leq 0$.

7. a) Suppose M is symmetric and homogeneous with $t_M(0) > 0$ or with $t_M(\infty) < \infty$, then

$$\lim_{p\to-\infty} M_p(a, b) = a \wedge b \qquad \text{and} \qquad \lim_{p\to\infty} M_p(a, b) = a \vee b.$$

b) In particular, this holds for H_p.
c) If, in addition, M_p is isotone in p, then

$$\lim_{p\to-\infty} {}_pM(a, b) = a \wedge b \qquad \text{and} \qquad \lim_{p\to\infty} {}_pM(a, b) = a \vee b\,.$$

d) In particular, this holds for L_p.

8. a) Show that ${}_pM$ is isotone in p if $g(p) := \log M(a^p, b^p)$ is always convex, since then $g(p+1) - g(p)$ increases with p. (See Beckenbach [50].)
b) Use Cauchy's inequality to show that this holds for

$${}_pA(a, b) = L_p(a, b) = \frac{a^p + b^p}{a^{p-1} + b^{p-1}}\,.$$

9. a) Establish the assertions about Stolarsky's means.
b) Show that

$$\sqrt{\sqrt{ab}\left(\frac{\sqrt{a}+\sqrt{b}}{2}\right)^2} \leq \mathcal{L}(a, b) \leq H_{1/2}(a, b)\,.$$

c) Show that

$$\frac{x-1}{\log x} = \prod_{k=1}^{\infty} \frac{1 + x^{2^{-k}}}{2}$$

and deduce that

$$\mathcal{L}(a, b) = \prod_{k=1}^{\infty} \frac{a^{2^{-k}} + b^{2^{-k}}}{2}\,.$$

10. a) Show that $\mathcal{L}_p(a, b)$ is isotone in p by applying Exercise 5a) and observing that (8.1.17) becomes $\mathcal{I}(a, b) \geq \mathcal{L}(a, b)$. [This in turn follows by calculus from $(t-1)^2 \geq t \log^2 t$, $t > 1$.]

b) Show that $\mathcal{I}_p(a, b)$ is isotone in p This can be done by showing that (8.1.17) becomes

$$\frac{\Phi(a)\log(a) - \Phi(b)\log(b)}{a-b} + 1 \geq \left[\frac{\Phi(a) - \Phi(b)}{a-b}\right]^2$$

which again reduces to $(t-1)^2 \geq t \log^2 t$.
c) The generalized mean $E_{r,s}$ is defined by

$$\text{(8.1.18)} \qquad E_{r,s}(a, b) := \left[\frac{s(a^r - b^r)}{r(a^s - b^s)}\right]^{1/(r-s)}$$

and extended appropriately on the boundary (as in Leach and Scholander [78]). Show that each $E_{r,s} = (S_p)_q$ for some p and q.
Let $\lambda(r) := \log|(a^r - 1)/r|$ so that $\dot{\lambda}(r) = \log \mathcal{I}_r(a, 1)$. By b) $\lambda(r)$ is convex. Thus for $s > r$,

$$\log E_{s,r}(a, 1) = \frac{\lambda(s) - \lambda(r)}{s - r} \geq \log \mathcal{I}_r(a, 1)$$

and $E_{s,r}$ increases in r and s because $E_{r,r} = \mathcal{I}_r$.
d) The mean

$$\text{He}(a, b) := E_{3/2,1/2}(a, b) = \frac{a + b + \sqrt{ab}}{3} = \frac{2}{3}A + \frac{1}{3}G$$

is very classical and is called *Heronian mean.*
e) Show that if $-1 \leq p \leq \frac{1}{2}$ or $p \geq 2$, then

$$\text{(8.1.19)} \qquad S_p(a, b) \leq H_{(p+1)/3}(a, b)$$

with the inequality reversed when $p \leq -1$ or $\frac{1}{2} \leq p \leq 2$. Moreover (8.1.19) fails if $(p+1)/3$ is replaced by any smaller number (larger in the reversed case). (See Stolarsky [80] for details.)
f) Show that $\mathcal{L}_p$ and $\mathcal{I}_p$ tend to $\vee$ as p tends to infinity.
g) Use the condition of Exercise 8a) to show that ${}_p\mathcal{L}$ is isotone in p.
h) Show that $E_{p,p-1} = {}_p\mathcal{L} \geq \mathcal{L}_p$ for $p \geq 1$ and so $E_{r,s} \geq \mathcal{L}_r$ for $r > s > 0$.
i) Show that

i) $(E_{r,s})_{-1} = E_{-r,-s}$
ii) $E_{r,s} = E_{s,r}$
iii) $E_{r,t}^{r-t} = E_{r,s}^{r-s} E_{s,t}^{s-t}$.

11. Prove Proposition 8.4 on the composition of means.

12. Let q be a nonnegative function satisfying

i) $q(1) = 1$
ii) $1 \wedge x < q(x) < x \vee 1 \qquad x \neq 1$.

a) Then

$$\bar{M}(x, y) := xq\left(\frac{y}{x}\right) \vee yq\left(\frac{x}{y}\right)$$

and

$$\underline{M}(x, y) := xq\left(\frac{y}{x}\right) \wedge yq\left(\frac{x}{y}\right)$$

are (possibly discontinuous), homogeneous, symmetric, strict means.

b) Suppose in addition that

iii) $q(x) = xq\left(\frac{1}{x}\right)$.

Then

$$\bar{M}(1, x) = q(x) = t_{\bar{M}}(x)\,.$$

Hence if we take an arbitrary (even analytic) function satisfying iii) with $1 < q(x) < x$ for $x > 1$, there is a strict, homogeneous mean with $t_M = q$.

c) Let $q(x) := \begin{cases} \dfrac{1+3x}{4} & x > 1, \quad x \text{ rational} \\ \dfrac{1+x}{2} & \text{otherwise} \end{cases}$.

Then $\bar{M}$ is a densely discontinuous mean which is not ultimately monotone. Moreover $\bar{M}$ lies between two continuous means.

13. Let $P_n(a, b) := \left(\sum_{k=0}^{n} c_k a^k b^{n-k}\right)^{1/n} \qquad c_k \ge 0, \quad \sum_{k=0}^{n} c_k = 1\,.$

Then P_n is a homogeneous strict mean which is symmetric if and only if $c_k = c_{n-k}$.

14. If M is a continuously differentiable mean then $M_0 := \lim_{p\to 0} M_p$ exists and is given by

$$M_0(a, b) = a^q b^{1-q}$$

where $q := (\partial M/\partial a)(1, 1)$.
Hint: Use L'Hôpital,s rule.

8.2 *EQUIVALENCE OF MEANS*

Let $\Phi\colon \mathbb{R}^+ \to \mathbb{R}^+$ be continuous. We say that a mean M *dominates* a mean N if

$$M(\Phi(a), \Phi(b)) = \Phi(N(a, b)) \qquad a, b > 0$$

and we write $M >_\Phi N$ or $M > N$. If M and N dominate each other, we call M and N *equivalent*. Since *domination* is transitive, this is an equivalence relation which we write $\sim$. Unfortunately most of our results demand that we consider more restrictive notions of equivalence, so we require that Φ be one to one from now on. Hence Φ is monotone.

Theorem 8.1

Suppose that M and N are two means with $M >_\Phi N$.

(*a*) Suppose that N is homogeneous. For each $t > 0$, consider $g_t(x) := \Phi(t\Phi^{-1}(x))$. Then g_t is isotone and

(8.2.1) $$M(a, b) = g_t^{-1} M(g_t(a), g_t(b))$$

for each a, b in rng (Φ).

(*b*) Suppose that $M := A$. Then

$$\Phi = \alpha\iota^p + \beta \qquad \alpha > 0,\ p \ne 0$$

and $N = H_p$, $p \ne 0$.

(*c*) Suppose that $M := G$. Then either

$$\Phi = \iota^p \qquad p \ne 0$$

or

$$\Phi = \alpha e^{\beta\iota^p} \qquad \alpha > 0, \quad p \ne 0$$

and $N = H_p$, $p \in \mathbb{R}$.

(*d*) It follows that the only homogeneous means equivalent to A are the Holder p means (H_p, $p \ne 0$) and the only homogeneous mean equivalent to G is G.

Proof

(*a*) By homogeneity of N we have, for $t > 0$,

$$\Phi^{-1}M(\Phi(ta), \Phi(tb)) = t\Phi^{-1}M(\Phi(a), \Phi(b))$$

and (8.2.1) follows. Moreover g_t is isotone as a composition of two co-monotone functions.

(*b*) Now (8.2.1), with $M := A$, becomes

$$2g_t\left(\frac{a+b}{2}\right) = g_t(a) + g_t(b) \qquad a, b \in \operatorname{rng}(\Phi)\,. \tag{8.2.2}$$

This is solved [Exercise 1a)] by

$$g_t(x) = a(t)x + b(t) \qquad x \in \operatorname{rng}(\Phi) \tag{8.2.3}$$

for some $a(t)$ and $b(t)$ in $\mathbb{R}$. Thus

$$\Phi(tx) = a(t)\Phi(x) + b(t) \qquad x, t > 0\,.$$

Now Exercise 1b) shows that this is solved by

$$\Phi = \begin{cases} \alpha\iota^p + \beta \\ \alpha \log + \beta \end{cases} \qquad p \neq 0\,. \tag{8.2.4}$$

Since Φ is positive, we must have $\Phi = \alpha\iota^p + \beta$, $\alpha > 0$, and N is as claimed.

(*c*) In this case we have

$$\sqrt{g_t(a)g_t(b)} = g_t(\sqrt{ab}) \qquad a, b \in \operatorname{rng}(\Phi)\,. \tag{8.2.5}$$

Let $h_t := \log(g_t \circ \exp)$. Then

$$h_t\left(\frac{a+b}{2}\right) = \frac{h_t(a) + h_t(b)}{2}\,.$$

As above $h_t(x) = a(t)x + b(t)$ and

$$\Phi(tx) = B(t)\Phi(x)^{a(t)} \tag{8.2.6}$$

for $B(t)$ positive. This is solved by

$$\Phi = \begin{cases} \alpha\iota^p \\ \alpha e^{c\iota^p} \end{cases} \qquad p \neq 0 \tag{8.2.7}$$

[as in Exercise 1c)]. If Φ is of the first type, $N = G$; while if Φ is of the second type, $N = H_p$, $p \neq 0$.

(*d*) Thus all H_p, $p \neq 0$, are equivalent and G dominates them all. $\square$

A more general program may be undertaken, based on Theorem 8.1(*a*). Unfortunately, without extra hypotheses, solutions of (8.2.1) are very hard to characterize. The following simple result is accessible.

Proposition 8.5

Suppose M is a homogeneous, strict mean with $M >_h N$ for some isotone h, and suppose $t_N(0) = 0$. Then $t_M(0) = 0$.

Proof. Since $h(N(a,1)) = M(h(a), h(1))$, we have $h(0) = h(N(0,1)) = M(h(0), h(1))$. This is only possible if $h(0) = 0$, $h(0) = h(1)$, or $h(0) = \infty$. Since h is strictly increasing, only $h(0) = 0$ can occur. Thus $h(0) = 0 = M(0, h(1))$. Since M is homogeneous, $t_M(0) = 0$ as claimed. $\square$

As an example we see that $H_p >_h \mathrm{AG}$, $p > 0$ (AG is the Gaussian AGM) is impossible for h isotone, as is $L_p >_h \mathrm{AG}$ with $p \geq 1$. These considerations suggest that we can say more if h is required to be onto. We will write $M \simeq N$ if $M >_h N$ for some one-to-one mapping h of $\mathbb{R}^+$ onto $\mathbb{R}^+$ [so that h must be (strictly) isotone with $h(0) = 0$, $h(\infty) = \infty$ or (strictly) antitone with $h(0) = \infty$, $h(\infty) = 0$]. This is an equivalence relation stronger than $\sim$, and we call it *strong equivalence*. We will only consider strong equivalence of homogeneous means. If we let $g_t := h(th^{-1})$, g_t is surjective and we observe that (8.2.1) becomes

$$g_t(M(a,b)) = M(g_t(a), g_t(b)) \qquad a, b > 0\,.$$

Since M is homogeneous, we may replace g_t by $h_t := g_t/g_t(1)$. Then $h_t(1) = 1$ and

$$h_t(M(a,b)) = M(h_t(a), h_t(b)) \qquad a, b > 0\,. \tag{8.2.8}$$

In the next lemma we give several conditions for (8.2.8) to have only the trivial solutions (normalized). Under these conditions we have $g_t = c(t)\iota$ and

$$h(tx) = c(t)h(x) \qquad t, x > 0\,. \tag{8.2.9}$$

Then Exercise 1b) shows $h = \alpha\iota^p$, $\alpha > 0$, $p \neq 0$, and it follows that the only homogeneous means strongly equivalent to M are M_p, $p \neq 0$. Thus we have determined the strong equivalence class of M in the cases covered by the next result.

Lemma 8.1

Suppose M is a homogeneous strict mean.

(*a*) The following two conditions imply that (8.2.8) only has the trivial solution when $h_t(1) = 1$.

(*i*) M is ultimately monotone and
(*ii*) $h_t(\bar{a}) = \bar{a}$ for some $\bar{a} \neq 1$, $\bar{a} > 0$.

(*b*) (*i*) (*ai*) holds if M is isotone (or piecewise monotone), while
(*ii*) (*aii*) holds if M is differentiable and (1) $\dot{t}_M$ has a unique positive zero, $\bar{a} \neq 1$ and h is differentiable; or (2) $t_M(\mathbb{R}^+) \subsetneq \mathbb{R}^+$.

Proof.

(*a*) Given that $\bar{a}$ and 1 are distinct positive fixed points of h_t, it follows from (8.2.8) and continuity that $\{c > 0 | h_t(c) = c\}$ is a closed interval C. We show that $s := \sup C$ is ∞. If not we argue as follows.

For any $c < s$ in C, $M(c, s) < s$. Hence $M(c, s + \varepsilon) < s$ for some $\varepsilon > 0$. But $M(s, s + \varepsilon) > s$. Thus $M(c, s + \varepsilon) = s$ for some $c < s$, c in C, $\varepsilon > 0$. Then for $n = 1, 2, 3, \ldots,$

$$s = h_t^n(s) = M(h_t^n(c), h_t^n(s + \varepsilon)) = M(c, h_t^n(s + \varepsilon)) .$$

(Here $h^n := h^{n-1} \circ h$ denotes iterated composition.)

Let $b_n := c^{-1} h_t^n(s + \varepsilon)$. Then, as $b_1 \neq b_0$ (because $s + \varepsilon \not\in C$), b_n is a strictly monotone sequence, since h_t is strictly isotone. If $\{b_n\}$ were bounded above, the limit point would be a member of C larger than s. Thus b_n increases without bound and also $t_M(b_n) = s/c$. This violates monotonicity of M at infinity. The proof that $\inf C = 0$ is left as Exercise 2b).

(*b*) We consider (*ii*). If h and M are differentiable, we have from (8.2.8)

$$\dot{t}_M(h_t(x))\dot{h}_t(x) = \dot{h}_t(t_M(x))\dot{t}_M(x) .$$

Since h_t is strictly increasing, we have $\dot{t}_M(h_t(\bar{a})) = 0$ and $h_t(\bar{a}) = \bar{a}$. If on the other hand t_M is not surjective, we argue as follows. Suppose $M(0, 1) > 0$. Then

$$h_t(M(0, 1)) = M(h_t(0), h_t(1)) = M(0, 1)$$

as $h_t(0) = 0$, and $M(0, 1) < 1$ is a second fixed point of h_t. Finally if $M(\infty, 1) < \infty$, we argue with M_{-1}. □

Condition (*ai*) holds for H_p, L_p, and S_p. Condition (2) of (*bii*) holds for H_p, $p \neq 0$; for L_p, $p \leq 0$ or $p \geq 1$; and for S_p, $p > 0$; while condition (1) holds for L_p, $p \geq 1$. (See Exercise 3.) It is reasonable, at least for computational purposes, to require that equivalence be defined by differentiable maps. If this is done, the results are more complete.

Comments and Exercises

Theorem 8.1 can be found in Wimp [84] in slightly different form. This is partly explained by the fact that $\exp[(\log x + \log y)/2] = G(x, y)$. For Hardy, Littlewood, and Polya [59] or Wimp [84] this means that $A >_{\log} G$. In a more formal development this is problematical since means are only defined on $(\mathbb{R}^+)^2$ and log is not always positive. Thus we rule out the second case in (8.2.4).

1. a) Show, using continuity of g_t, that (8.2.2) is solved as in (8.2.3). (Proofs without continuity assumptions can be found in Wimp [84] and elsewhere. More general results depend on the measurability of g_t.)

b) Let $\psi(x) := \Phi(x) - \Phi(1)$. Then ψ satisfies

$$\psi(tx) = a(t)\psi(x) + c(t)$$

for some $c(t)$ in $\mathbb{R}$. Then $\psi(t) = c(t)$ and thus $[a(x) - 1]/\psi(x) = [\psi(tx) - \psi(t) - \psi(x)]/\psi(t)\psi(x)$ is independent of x if $\psi(x) \neq 0$. Thus $\psi(xy) = c\psi(x)\psi(y) + \psi(x) + \psi(y)$. If $c = 0$, then $\psi(x) = C \log x$, while if $c \neq 0$, $\lambda(x) := c\psi(x) + 1$ solves $\lambda(xy) = \lambda(x)\lambda(y)$ whose solution is ι^p. Thus (8.2.4) holds.

c) Show that (8.2.6) has solutions only of form (8.2.7). *Hint*: Consider $\lambda(x) := \log[\Phi(x)] - \log[\Phi(1)]$. Then $\lambda(xt) = a(t)\lambda(x) + \lambda(t)$. Now proceed much as in b).

2. a) By considering M_{-1} show that if $M >_h N$, M strict and homogeneous, h isotone with $t_M(\infty) < \infty$, then $t_N(\infty) < \infty$.

b) Complete the proof of Lemma 8.1(*a*).

c) Complete the proof of Lemma 8.1(*b*).

3. a) Verify the final claims of this section.

b) Calculate the strong equivalence classes within $G_{r,s}$ and $E_{r,s}$.

4. a) If M is a symmetric, homogeneous, strict mean, then either $t_M(0) = 0$ or $t_M(\infty) = \infty$.

b) Similarly, suppose then that $M >_h N$ for some homogeneous N with h monotone. Show that 0 or ∞ lies in $\text{rng}(h)$.

8.3 *COMPOUND MEANS*

We now formalize the notion of a mean iteration. The Gaussian AGM and Archimedes' method provide the central examples. Let M and N be any two continuous means. Let $a > 0$ and $b > 0$ be given and consider the iteration

(8.3.1)
$$a_0 := a \qquad b_0 := b$$
$$a_{n+1} := M(a_n, b_n)$$
$$b_{n+1} := N(a_n, b_n) .$$

Under mild hypotheses, Theorem 8.2 shows that the iterates converge to a common limit, which we call the *compound* of M and N and denote by

$M \otimes N(a, b)$. We will also denote the entire iterative process by $[M, N]$. We say that M is *comparable* to N if one of the following holds:

(a) $M(a, b) \geq N(a, b)$ for $a, b > 0$
(b) $M(a, b) \leq N(a, b)$ for $a, b > 0$

or

(c) $M(a, b) \leq N(a, b)$ for $0 < a < b$

and

$N(a, b) \leq M(a, b)$ for $0 < b < a$.

When M and N are symmetric, c) cannot occur, and we say M and N are comparable. In the nonsymmetric case c) can occur, and then M is comparable to N but not conversely. In the next result comparability is only needed to establish monotonicity of the iterates. (See Exercise 1 and Theorem 8.8 of Section 8.7.)

Theorem 8.2

Let M and N be means with M comparable to N.

(*a*) Suppose that M or N is strict. Then $[M, N]$ converges and $M \otimes N$ is a mean which is strict if both M and N are.
(*b*) $M \otimes N$ is a homogeneous, symmetric, or isotone if each of M and N is.
(*c*) $M \otimes N$ is continuous, and the convergence is monotone and uniform on compact subsets of $\{(a, b) | a, b > 0\}$.

Proof

(*a*) Suppose that $a > b$ and that $M \geq N$. Then $a_1 = M(a, b) \geq N(a, b) = b_1$. Inductively suppose that $a_n \geq b_n$. Then

(8.3.2) $$a_n \geq M(a_n, b_n) = a_{n+1} \geq b_{n+1} = N(a_n, b_n) \geq b_n$$

and $\{a_n\}$ decreases while $\{b_n\}$ increases. Since each bounds the other, both sequences converge, say, to x and y, respectively. By continuity we have $x = M(x, y)$ and $y = N(x, y)$. Since M or N is strict, $x = y$. If $a \leq b$, we may have to exchange the roles of a_n and b_n. Thus $M \otimes N$ exists and satisfies

(8.3.3) $$M \wedge N \leq M \otimes N \leq M \vee N .$$

This finishes (*a*).

(*b*) The sequences $\{a_n\}$ and $\{b_n\}$ are in fact built by repeated composition of means. Thus $a_n = M_n(a, b)$ and $b_n = N_n(a, b)$ for means M_n and N_n. These means are symmetric, homogeneous, or isotone when M and N are, and so is the limit mean $M \otimes N$.
(*c*) Let $a, b > 0$ and $\varepsilon > 0$ be given. Pick n so that $|a_n - b_n| < \varepsilon/2$. Now M_n and N_n are continuous. So we may find $\delta > 0$ with $|M_n(a, b) - M_n(a', b')| < \varepsilon/2$ and $|N_n(a, b) - N_n(a', b')| < \varepsilon/2$ if $|a' - a| < \delta$ and $|b' - b| < \delta$, $(a', b' > 0)$. Again assume $a > b$ and $M \geq N$. Then

$$M \otimes N(a', b') \leq M_n(a', b') \leq M_n(a, b) + \frac{\varepsilon}{2} \leq N_n(a, b) + \varepsilon$$
$$\leq M \otimes N(a, b) + \varepsilon$$

and

$$M \otimes N(a', b') \geq N_n(a', b') \geq N_n(a, b) - \frac{\varepsilon}{2} \geq M_n(a, b) - \varepsilon$$
$$\geq M \otimes N(a, b) - \varepsilon .$$

Thus $M \otimes N$ is continuous. Finally, Dini's theorem shows that M_n and N_n must actually converge uniformly on compact subsets, since convergence is monotone. □

The key observation about $M \otimes N$ is the following 'invariance principle' which we have already used repeatedly in Chapters 1 and 2 to show that $AG(1, k') = \pi/2K$.

Theorem 8.3 (Invariance Principle)

Suppose that $M \otimes N$ exists. Then $M \otimes N$ is the unique, (continuous) mean Φ satisfying

(8.3.4) $$\Phi(M(a, b), N(a, b)) = \Phi(a, b)$$

for all $a, b > 0$.

Proof. Iteration of (8.3.4) shows that

$$\lim_{n \to \infty} \Phi(a_n, b_n) = \Phi(a, b) .$$

Thus

$$\Phi(a, b) = \Phi(M \otimes N(a, b), M \otimes N(a, b))$$

and since $\Phi(c, c) = c$, $\Phi = M \otimes N$. □

Observe that we need not verify that Φ is a mean, but only that $\Phi(x,x)=x$ for $x>0$ and that Φ is a continuous solution of (8.3.4).

EXAMPLE 8.1

(*a*) Let $M:=H_1$ and $N:=H_{-1}$. Then $H_1 \otimes H_{-1}=G$. Observe that $G(a,b):=\sqrt{ab}$ satisfies

$$G(H_1(a,b),H_{-1}(a,b))=\sqrt{\frac{a+b}{2}\,\frac{2ab}{a+b}}=\sqrt{ab}\qquad \Phi(a,b):=\sqrt{ab}.$$

Since $\sqrt{xx}=x$, we must have $H_1\otimes H_{-1}=G$.

(*b*) Let $M(a,b):=9ab^2/(a+2b)^2$ and $N(a,b):=(a+2b)/3$. Then

$$M^{1/3}(a,b)N^{2/3}(a,b)=a^{1/3}b^{2/3}\qquad \Phi(a,b):=a^{1/3}b^{2/3}$$

and again the invariance principle shows that $M\otimes N(a,b)=a^{1/3}b^{2/3}$.

(*c*) Let $H_1\otimes H_0=\mathrm{AG}:=A\otimes G$. Then for $a\geq b$,

$$A\otimes G(a,b)=a\mathrm{AG}\left(1,\frac{b}{a}\right)=\frac{a\pi}{2K'(b/a)}\qquad \Phi(a,b):=\frac{a\pi}{2K'(b/a)}$$

as Theorem 1.1 (second proof) shows by the invariance principle.

We now distinguish two better structured classes of mean iterations.

Definition 8.2

Let M and N be symmetric means.

(*a*) Suppose M and N are comparable. Then we write

$$M\otimes_g N:=M\otimes N \qquad\text{and}\qquad [M,N]_g:=[M,N].$$

We call these *Gaussian mean iterations* and call $\otimes_g$ the *Gaussian product*.

(*b*) Consider the iteration: $a_0:=a>0$, $b_0:=b>0$, and

$$a_{n+1}:=M(a_n,b_n)$$
$$b_{n+1}:=N(a_{n+1},b_n).$$

We denote the iteration by $[M,N]_a$ and the limit by $M\otimes_a N$. We call these *Archimedean mean iterations* and call $\otimes_a$ the *Archimedean product*.

The existence of $M\otimes_g N$ is guaranteed by Theorem 8.2. For $M\otimes_a N$ existence comes from the next result.

Proposition 8.6

Let M and N be symmetric means. Suppose that M is strict. Then $M\otimes_a N$ exists and

$$M\otimes_a N=M\otimes N^*$$

where $N^*(a,b):=N(M(a,b),b)$. So by Theorem 8.3 $M\otimes_a N$ is the unique continuous mapping ψ satisfying

$$\psi(M(a,b),N^*(a,b))=\psi(a,b)$$

with $\psi(x,x)=x$ for $x>0$.

In consequence $M\otimes_a N$ is a continuous mean which is strict, homogeneous, or isotone whenever both M and N are.

Proof. This follows from Theorem 8.3 since M is comparable to N^* (See Exercise 4.) □

The theorem makes no use of symmetry of M and N. However, this is critical to our further analysis of convergence rates. Finally, suppose that we are given a function M which satisfies (8.1.1) and (8.1.2) or (8.1.3), but only for $0<a<b$. We may extend M to a symmetric mean $\tilde{M}$ via

$$\tilde{M}(a,b):=M(a\wedge b,a\vee b).\tag{8.3.5}$$

Similarly we can extend a function defined only on $0<b<a$ by using $M(a\vee b,a\wedge b)$. The new mean is homogeneous or strict when M is. Thus in some of our future iterations we will consider means only defined on the 45° sectors (Exercise 3 among others). Moreover, if we have two comparable means on $0<b<a$, the extensions are comparable so that our convergence results apply. Note also that in the definition of comparability we excluded the possibility that $M\leq N$ for $0<b<a$ while $N\leq M$ for $0<a<b$. In this case the iterates oscillate, and combining two steps results in a comparable iteration. We call such iterates *partially comparable*.

Comments and Exercises

Our treatment is a synthesis and extension of that in Schoenberg [77, 82], Lehmer [71], and Foster and Phillips [84*b*] among others. The term compound is due to Lehmer [71]. In general it is very hard to determine $M\otimes N$, but easy to verify a limit once one has found it. Schoenberg [77] gives a geometric proof of the limit of the AGM due to Jacobi.

1. a) Let M and N be strict means. Then $[M,N]$ converges and $M\otimes N$ is a strict (continuous) mean.

Hint: $\{a_n \vee b_n\}$ and $\{a_n \wedge b_n\}$ are monotone sequences, and so $a_n \vee b_n$ decreases to x and $a_n \wedge b_n$ increases to y. One may suppose $x = (M \vee N)(x, y)$. Thus $x = y$ by Proposition 8.4 and $M \otimes N$ exists. Since $M \wedge N \le M \otimes N \le M \vee N$, the limit is a strict mean.

b) $M \otimes N$ is symmetric or homogeneous when M and N are.

2. a) Let M be a strict mean. Then

$$M \otimes \vee = \vee \otimes M = \vee .$$

b) Show that

$$(M \otimes N)_f = M_f \otimes N_f$$

where as before $M_f(a, b) := f^{-1}M(f(a), f(b))$.

c) In particular a) and b) show that

$$M \otimes \wedge = \wedge \otimes M = \wedge .$$

d) If M and N are symmetric, then

$$M \otimes N = N \otimes M .$$

[More generally, $N \otimes M(a, b) = M \otimes N(b, a)$.] Thus

$$M \otimes_g N = N \otimes_g M .$$

3. (*Carlson's log*) Define means $M(a, b) := \sqrt{a \cdot (a+b)/2}$ and $N(a, b) := \sqrt{[(a+b)/2] \cdot b} = M(b, a)$. Show that

$$M \otimes N(a, b) = \sqrt{\frac{a^2 - b^2}{2 \log (a/b)}} \qquad \text{for } a \neq b .$$

Hence [using Exercise 2b)],

$$M_{1/2} \otimes N_{1/2} = \mathcal{L} .$$

Explicitly, if

$$a_{n+1} := \frac{a_n + \sqrt{a_n b_n}}{2} \qquad \text{and} \qquad b_{n+1} := \frac{b_n + \sqrt{a_n b_n}}{2}$$

then the limit is

$$\frac{b - a}{\log b - \log a} .$$

Note that this is neither a Gaussian nor an Archimedean iteration.

4. Prove Proposition 8.6 from Theorem 8.3. Note that in this setting $M \le N^*$ for $0 < a < b$ and $M \ge N^*$ for $0 < b < a$.

5. a) Show that given strict symmetric means M and N,

$$M \otimes_a N(b, N(a, b)) = N \otimes_a M(a, b) .$$

b) Show that in the special case in which $M = N$ the limit $M \otimes_a M := \Phi$ is characterized by

$$\Phi(a, b) = \Phi(b, M(a, b)) .$$

c) Show [using b) or otherwise] that

i) $A \otimes_a A(a, b) = \dfrac{a + 2b}{3}$

ii) $G \otimes_a G(a, b) = a^{1/3} b^{2/3}$

iii) $H_p \otimes_a H_p(a, b) = \left(\dfrac{a^p + 2b^p}{3}\right)^{1/p} \qquad p \neq 0 .$

6. For any function Q let $\tilde{Q}(a, b) := Q(b, a)$. Prove that for any means M and N,

$$M \tilde{\otimes} N = \tilde{N} \otimes \tilde{M}$$

and

$$M \otimes_a N(b, N(b, a)) = \tilde{N} \otimes_a \tilde{M}(a, b) .$$

8.4 *CONVERGENCE RATES AND SOME EXAMPLES*

In this section we show that Gaussian iterations typically converge quadratically and Archimedean iterations sublinearly. We also give some more examples of Gaussian and Archimedean iterations for which we can calculate the limit.

EXAMPLE 8.2 (ARCHIMEDES' METHOD)

(*a*) Let a_n denote the area of a regular $m \cdot 2^n$-gon inscribed in a unit circle. Let b_n denote the area of the circumscribed regular $m \cdot 2^n$-gon. It is easily verified that $a_{n+1} = \sqrt{a_n b_n}$ and $b_{n+1} = 2a_{n+1}b_n/(a_{n+1} + b_n)$ while $a_0 = \frac{1}{2} m \sin (2\pi/m)$ and $b_0 = m \tan (\pi/m)$. Thus we geometrically verify that a_n and b_n tend to π. This gives $G \otimes_a H_{-1}(a_0, b_0) = \pi$ or, on using homogeneity and replacing $2\pi/m$ by θ, (8.4.1) $$G \otimes_a H_{-1}\left(\sin\theta, 2\tan\left(\frac{\theta}{2}\right)\right) = \theta .$$

There is no need for m to be integral and (8.4.1) holds for all $0<\theta<\pi$.

(*b*) Consider now the same process but using circumscribed and inscribed perimeters a_n and b_n. Now we have $a_{n+1} = 2a_nb_n/(a_n+b_n)$ and $b_{n+1} = \sqrt{a_{n+1}b_n}$ while $a_0 = 2m\tan(\pi/m)$ and $b_0 = 2m\sin(\pi/m)$. Then a_n and b_n tend to 2π and

(8.4.2) $$H_{-1} \otimes_a G(\tan\theta, \sin\theta) = \theta .$$

This is pursued further in Exercises 1 and 2. □

A complete analysis of the iteration of Schwab, Borchardt, Pfaff, and Gauss is in Miel [83]. The central observation is:

Theorem 8.4 (Schwab–Borchardt)

(8.4.3) $$A \otimes_a G(a,b) = \begin{cases} \dfrac{\sqrt{b^2-a^2}}{\arccos(a/b)} & 0 \le a < b \\ a & a = b \\ \dfrac{\sqrt{a^2-b^2}}{\operatorname{arccosh}(a/b)} & 0 < b < a \end{cases} .$$

Proof. Schwab established the first case by geometric arguments which Schoenberg [82] reproduces. Given the formulae, it is simpler to use the invariance principle. Since $a_{n+1}^2 - b_{n+1}^2 = (a_n^2 - b_n^2)/4$, this reduces to showing that

(8.4.4) $$\begin{aligned} 2\arccos\left(\frac{a_{n+1}}{b_{n+1}}\right) &= \arccos\left(\frac{a_n}{b_n}\right) \qquad a_n < b_n \\ 2\operatorname{arccosh}\left(\frac{a_{n+1}}{b_{n+1}}\right) &= \operatorname{arccosh}\left(\frac{a_n}{b_n}\right) \qquad a_n > b_n . \end{aligned}$$

Since $a_{n+1}/b_{n+1} = \sqrt{(a_n/b_n+1)/2}$, this is just the half-angle formula for cos or cosh. □

We now turn to study rates of convergence for Gaussian and Archimidean means.

Theorem 8.5

Let M and N both be continuously differentiable symmetric means and suppose that at least one is strict.

(*a*) Consider the Archimedean iteration $[M, N]_a$. Then, if $a_n \neq b_n$,

(8.4.5) $$\lim_{n\to\infty} \frac{a_{n+1}-b_{n+1}}{a_n-b_n} = \frac{1}{4} .$$

(*b*) Consider the Gaussian iteration $[M, N]_g$ for comparable M and N.

(*i*) Then, if $a_n \neq b_n$,

(8.4.6) $$\lim_{n\to\infty} \frac{a_{n+1}-b_{n+1}}{a_n-b_n} = 0 .$$

(*ii*) Suppose, in addition, that M and N are twice continuously differentiable. Then, if $a_n \neq b_n$,

(8.4.7) $$\lim_{n\to\infty} \frac{|a_{n+1}-b_{n+1}|}{|a_n-b_n|^2} = \frac{|M_{11}(s,s)-N_{11}(s,s)|}{2}$$

where $s := M \otimes_g N(a,b)$.

Proof. Since $M(c,c)=c$ for all c, we must have $M_{,1}(c,c) + M_{,2}(c,c) = 1$ for all c. (Here $M_{,i}$ denotes the partial derivative with respect to the ith variable.) Since M and N are symmetric, it follows that $M_{,i}(c,c) = N_{,i}(c,c) = \frac{1}{2}$, $i = 1, 2$.

(*a*) Let $s := (M \otimes_a N)(a,b)$. The mean value theorem gives

(8.4.8) $$a_{n+1} - s = \tfrac{1}{2}(a_n - s) + \tfrac{1}{2}(b_n - s) + o(a_n - s) + o(b_n - s)$$

and since $b_{n+1} = N(a_{n+1}, b_n)$,

(8.4.9) $$\begin{aligned} b_{n+1} - s &= \tfrac{1}{2}(a_{n+1} - s) + \tfrac{1}{2}(b_n - s) + o(a_{n+1} - s) + o(b_n - s) \\ &= \tfrac{1}{4}(a_n - s) + \tfrac{3}{4}(b_n - s) + o(a_n - s) + o(b_n - s) . \end{aligned}$$

Thus

$$a_{n+1} - b_{n+1} = \tfrac{1}{4}(a_n - b_n) + o(a_n - s) + o(b_n - s)$$

and (*a*) follows.

(*b*) (*i*) Similarly, (8.4.8) still holds, and also

(8.4.10) $$b_{n+1} - s = \tfrac{1}{2}(a_n - s) + \tfrac{1}{2}(b_n - s) + o(a_n - s) + o(b_n - s) .$$

Thus

$$a_{n+1} - b_{n+1} = o(a_n - s) + o(b_n - s) = o(a_n - b_n)$$

(since s lies between a_n and b_n). This gives (b).

(ii) Given one more derivative, we have

$$a_{n+1} - s = \tfrac{1}{2}(a_n - s) + \tfrac{1}{2}(b_n - s) + \tfrac{1}{2}M_{11}(s, s)(a_n - b_n)^2 + o(a_n - b_n)^2$$

and a similar formula for b_n. Subtraction gives (ii). Here we have used $\nabla^2 M(s, s)(a_n - s, b_n - s)^2 = M_{11}(s, s)(a_n - b_n)^2$. [Exercise 7d).] □

Considerably more can be said if M and N are two or three times continuously differentiable. (See Foster and Phillips [84*b*].) In addition the convergence in each case is uniform. For our purposes Theorem 8.5 suffices. In particular, Archimedean iterations characteristically converge linearly and Gaussian iterations super linearly (quadratically if twice differentiable). In light of Jacobi-type methods in the theory of equations, this may seem counterintuitive. Exercise 3c) shows that (8.4.6) may fail if M and N are not differentiable. The theorem justifies our separating Gaussian and Archimedean iterations. While symmetry is central to our convergence arguments, it is not always essential, all that is really needed in Theorem 8.5 is that the two means have the same gradients on the diagonal. (See Exercise 11.) Also, (8.4.7) shows that better than quadratic convergence is possible only if $M_{11} = N_{11}$. (See Exercise 7.) Additional information is given in Exercise 11.

Finally, let us say that two iterations are *equivalent* ($[M, N] \sim_h [M', N']$) if $M \sim_h M'$ and $N \sim_h N'$. *Strong equivalence* is similarly defined. Clearly equivalence of iterations implies equivalence of the limits, but not conversely. Indeed, if the mapping h is continuously differentiable, the rates of convergence must be the same. (See Exercise 8.)

Comments and Exercises

Some of the Archimedean considerations are discussed again in Chapter 11. If we take $m := 6$ in Example 8.2(b), we have a recursive version of Archimedes' original method. (See also Edwards [79] and Phillips [81].)

1. a) Show that (8.4.1) and (8.4.2) are consistent with the general formula of Exercise 5a) of Section 8.3.

b) Show directly that in both (a) and (b) of Example 8.2 we have $a_{n+1} - b_{n+1} \sim \tfrac{1}{4}(a_n - b_n)$. This illustrates why computation of any large number of digits of π by this method is impractical.

c) Show that in both cases $(a_n + 2b_n)/3 =: d_n$ satisfies

$$\frac{d_{n+1} - \lim d_n}{d_n - \lim d_n} \to \frac{1}{16} \qquad \text{as} \qquad n \to \infty .$$

2. a) Show that changes of variables cause no problems for Gaussian or Archimedean iterations, that is,

i) $(M \otimes_g N)_f = M_f \otimes_g N_f$

ii) $(M \otimes_a N)_f = M_f \otimes_a N_f$.

b) Show that (8.4.2) implies that

$$A \otimes_a G(x, 1) = \frac{\sqrt{1 - x^2}}{\arccos x} \qquad 0 \le x < 1 .$$

Hint: Let $x := \cos\theta$ in (8.4.2) and use aii).

c) Rederive Theorem 8.4 from b).

The next exercise shows a class of means which is closed under the Gaussian product. Contrast this with the Gaussian product of Holder means.

3. Let $Q_t(a, b) := t(a \vee b) + (1 - t)(a \wedge b)$ for $0 \le t \le 1$.

a) Show that Q_t is a homogeneous, symmetric, isotone mean which is strict for $0 < t < 1$.

b) Show that for $t \ge s$,

$$Q_t \otimes_g Q_s = Q_{s/[s+(1-t)]} .$$

This may easily be done by the invariance principle. Alternatively, suppose $a > b > 0$ and observe that the limit must be linear.

c) Show that $|a_n - b_n| = (t - s)^n |a - b|$.

d) Show that $Q_t \otimes_a Q_s = Q_t \otimes_g Q_{st}$.

4. Let M and N be symmetric, homogeneous means.

a) Show that $M \otimes_g N = G$ if and only if $N = M_{-1}$.

b) Show that $M \otimes_g N = A$ if and only if $N = 2A - M$. Note that M is a mean if and only if $2A - M$ is.

c) Characterize $M \otimes_g N = H_p$.

d) Show that if $M(a, b) := \sqrt{(a - b)^2 + ab}$, then

$$M \otimes_g G = H_2 .$$

a) Show that f_5 to f_{10} are symmetric, homogeneous means which are not differentiable on the diagonal. Thus Theorem 8.5(a) does not apply.
b) Show that $f_7 \otimes_g f_8 = A$, and that $[f_7, f_8]_a$ converges sublinearly for $a < b$ but quartically for $a > b$.
c) Show that $f_8 \otimes_g f_7(\frac{1}{2}, 1) = \frac{3}{4}$, and that we have one-step termination—which cannot happen for strictly comparable means.

These means were originally defined by the Greeks in terms of proportions. For $j := 1$ to 10, respectively, $x := f_j(a, b)$ solves

$$(1)\ \frac{x - \underline{m}}{\overline{m} - x} = \frac{\overline{m}}{\overline{m}} \qquad (2)\ \frac{x - \underline{m}}{\overline{m} - x} = \frac{\underline{m}}{x}$$

$$(3)\ \frac{x - \underline{m}}{\overline{m} - x} = \frac{\underline{m}}{\overline{m}} \qquad (4)\ \frac{x - \underline{m}}{\overline{m} - x} = \frac{\overline{m}}{\underline{m}}$$

$$(5)\ \frac{x - \underline{m}}{\overline{m} - x} = \frac{x}{\overline{m}} \qquad (6)\ \frac{x - \underline{m}}{\overline{m} - x} = \frac{\overline{m}}{x}$$

$$(7)\ \frac{\overline{m} - \underline{m}}{\overline{m} - x} = \frac{\overline{m}}{\overline{m}} \qquad (8)\ \frac{\overline{m} - \underline{m}}{x - \underline{m}} = \frac{\overline{m}}{\underline{m}}$$

$$(9)\ \frac{\overline{m} - \underline{m}}{\overline{m} - x} = \frac{\overline{m}}{x} \qquad (10)\ \frac{\overline{m} - \underline{m}}{x - \underline{m}} = \frac{x}{\underline{m}}$$

d) Verify that $x = f_j(a, b)$ in each case.
e) Verify that these are the only such means.

8.5 *CARLSON'S INTEGRALS AND MORE EXAMPLES*

This section is largely given to a description of a unified approach to Gauss's and Borchardt's algorithms due to Carlson [71]. It shows both the possibilities and the limitations of looking for iterative methods based on a more general hypergeometric transformation.

Let us consider the integral

$$R(\alpha; \delta, \delta'; x^2, y^2) := \frac{1}{\beta(\alpha, \alpha')} \int_0^\infty t^{\alpha'-1}(t + x^2)^{-\delta}(t + y^2)^{-\delta'}\, dt \tag{8.5.1}$$

where $\alpha + \alpha' = \delta + \delta'$; $\mathrm{re}(\alpha)$, $\mathrm{re}(\alpha') > 0$, and β is the beta function. (The prime is not complementation in this context.) Then obviously

$$R(\alpha; \delta, \delta'; x^2, y^2) = R(\alpha; \delta', \delta; y^2, x^2) \tag{8.5.2}$$

and R is homogeneous of degree $-\alpha$ in x^2 and y^2. (See Exercise 1.) We are interested in

$$C_{ij} := F_i \otimes F_j \qquad i, j = 1, 2, 3, 4 \tag{8.5.3}$$

where the means F_i, $i = 1, 2, 3, 4$, are given by

$$F_1(a, b) := \frac{a + b}{2} \qquad F_2(a, b) := \sqrt{ab}$$

$$F_3(a, b) := \sqrt{\frac{a + b}{2}\, a} \qquad F_4(a, b) := \sqrt{\frac{a + b}{2}\, b}\,.$$

Thus $C_{12} = \mathrm{AG}$, C_{34} produces Carlson's log (Exercise 3 of Section 8.3), and $C_{14} = A \otimes_a G$ leads to Borchardt's algorithm (Theorem 8.4).

Theorem 8.6 (Carlson)

Let $i, j = 1, 2, 3, 4$ with $i \neq j$.

(a) $[F_i, F_j]$ converges.

(b) $C_{ij}(a, b) = [R(\alpha; \delta, \delta'; a^2, b^2)]^{-1/2\alpha}$

where $(\alpha; \delta, \delta')$ is given by the (i, j)th entry Table 8.1.

(c) Convergence is linear except for $C_{12} = C_{21}$, which is AG, the limit of the Gaussian AGM.

TABLE 8.1

i	$j = 1$	$j = 2$	$j = 4$	$j = 3$
1	*	$(\frac{1}{2}; \frac{1}{2}, \frac{1}{2})$	$(\frac{1}{2}; \frac{1}{2}, 1)$	$(\frac{1}{4}; \frac{3}{4}, \frac{1}{2})$
2	$(\frac{1}{2}; \frac{1}{2}, \frac{1}{2})$	*	$(1; \frac{1}{2}, 1)$	$(1; \frac{3}{4}, \frac{1}{2})$
3	$(\frac{1}{2}; 1, \frac{1}{2})$	$(1; 1, 1)$	$(1; 1, 1)$	*
4	$(\frac{1}{4}; \frac{1}{2}, \frac{3}{4})$	$(1; \frac{1}{2}, \frac{3}{4})$	*	$(1; 1, 1)$

Since F_1 and F_2 are symmetric while $F_3(b, a) = F_4(a, b)$, up to exchange of δ and δ' the table is symmetric around the main diagonal because of (8.5.2). Boxes marked with $*$ correspond to trivial iterations.

Proof.

(a) Since $F_4 \le F_2 \le F_1 \le F_3$ for $0 < b < a$, each pair of means is partially comparable. By Proposition 8.4 on composition, each mean is strict. Thus Theorem 8.2 establishes (a).

(b) Let us denote $F_i(a, b)$ by f_i. Make, in (8.5.1), the substitution $t := s(s + f_2^2)/(s + f_1^2)$. Then

$$\frac{dt}{ds} = \frac{s^2 + 2sf_1^2 + f_1^2 f_2^2}{(s + f_1^2)^2} = \frac{(s + f_3^2)(s + f_4^2)}{(s + f_1^2)^2}$$

and

$$t + a^2 = \frac{(s + f_3^2)^2}{s + f_1^2} \qquad t + b^2 = \frac{(s + f_4^2)^2}{s + f_1^2}\,.$$

Thus

(8.5.4)

$$R(\alpha; \delta, \delta'; a^2, b^2) = \frac{1}{\beta(\alpha, \alpha')} \int_0^\infty s^{\alpha'-1}(s + f_1^2)^{\alpha-1}(s + f_2^2)^{\alpha'-1} \times (s + f_3^2)^{1-2\delta}(s + f_4^2)^{1-2\delta'}\, ds\,.$$

If we fix i and j, we can determine values of the parameters for which f_k, $k \neq i, j$, vanishes in (8.5.4). For example, with $i := 3$ and $j := 4$, we set $\alpha := \alpha' := 1$ and have

(8.5.5) $$R(1; \delta, \delta'; a^2, b^2) = R(1, 2\delta - 1, 2\delta' - 1; f_3^2, f_4^2)$$

where $\delta + \delta' = 2$. There is a unique value $\delta := 1$ so that (8.5.5) becomes invariant for f_3 and f_4. By Exercise 1b), $[R(1; 1, 1; a^2, b^2)]^{-1/2}$ is an invariant for $[F_3, F_4]$ to which Theorem 8.3 applies. Similarly, for $i := 1$ and $j := 2$, we set $\delta := \delta' := \frac{1}{2}$, which gives $\alpha + \alpha' = 1$ and

$$R(\alpha; \tfrac{1}{2}, \tfrac{1}{2}; a^2, b^2) = R(\alpha; 1 - \alpha, \alpha; f_1^2, f_2^2)\,.$$

The only possible invariant has $\alpha := \alpha' = \frac{1}{2}$, and by Exercise 1b), $[R(\frac{1}{2}; \frac{1}{2}, \frac{1}{2}; a^2, b^2)]^{-1}$ is an invariant for $[F_1, F_2]$. The rest of the table is similarly verified. [See Exercise 1c).]

(*c*) The convergence assertions are straightforward. [See Exercise 1d).] □

EXAMPLE 8.3. As observed before, C_{12}, C_{34}, and C_{14} have been previously identified. In Exercise 2 we indicate how to recover the previous forms of the limit. In particular Theorem 8.6 gives integral representations for these means. Now consider $i := 1$ and $j := 3$ (or similarly, $j := 1$ and $i := 4$). Suppose that $a > b$. Let

(8.5.6) $$1 - s^4 := \frac{t + b^2}{t + a^2}\,.$$

Then $s^4 = (a^2 - b^2)/(t + a^2)$ and

$$4(1 - s^4)^{-1/2}\, ds = -(a^2 - b^2)^{1/4}(t + a^2)^{-3/4}(t + b^2)^{-1/2}\, dt\,.$$

Since $\alpha := \frac{1}{4}$, $\delta := \frac{3}{4}$, and $\delta' := \frac{1}{2}$, we have $\alpha' = 1$, $\beta(\alpha, \alpha') = 4$, and

$$R\left(\frac{1}{4}; \frac{3}{4}, \frac{1}{2}; a^2, b^2\right) = \frac{1}{4}\int_0^\infty (t + a^2)^{-3/4}(t + b^2)^{-1/2}\, dt = (a^2 - b^2)^{-1/4}\int_0^{(1-b^2/a^2)^{1/4}} (1 - s^4)^{-1/2}\, ds\,.$$

Recall that the *arclemniscate sine* is

$$\operatorname{arcsl} x := \int_0^x (1 - s^4)^{-1/2}\, ds \qquad x^2 \le 1$$

and gives the arc length of the lemniscate ($r^2 = \cos 2\theta$) from the origin to the point with radial position x. (See also Theorem 1.7.) Thus

(8.5.7) $$C_{13}(a, b) = \frac{\sqrt{a^2 - b^2}}{[\operatorname{arcsl}(1 - b^2/a^2)^{1/4}]^2} \qquad 0 \le b < a\,.$$

Similarly,

(8.5.8) $$C_{13}(a, b) = \frac{\sqrt{b^2 - a^2}}{[\operatorname{arcslh}(b^2/a^2 - 1)^{1/4}]^2} \qquad 0 < a < b$$

where the *hyperbolic arclemniscate* is defined by

$$\operatorname{arcslh} x := \int_0^x (1 + s^4)^{-1/2}\, ds\,.$$

[See Exercise 2d).] Observe that $\sqrt{2}C_{13}^{-1/2}(1, 0) = K(1/\sqrt{2})$, by Theorem 1.7.

EXAMPLE 8.4 (ARCHIMEDEAN MEANS) Let us consider $H_p \otimes_a H_q$ for $p, q = \pm 1, 0$. Then the previous exercise and Exercise 5 of Section 8.3 show that it suffices to consider $H_1 \otimes_a H_1$, $H_1 \otimes_a H_0$, and $H_1 \otimes_a H_{-1}$. Exercise 5c) of Section 8.3 gives $H_1 \otimes_a H_1(a, b) = (a + 2b)/3$ while $H_1 \otimes_a H_0$ is Borchardt's algorithm. It remains to study $H_1 \otimes_a H_{-1}$. With $\alpha := \beta := \frac{1}{2}$, this is a special case of the mean iteration $a_0 := a > 0$ and $b_0 := b > 0$,

$$a_{n+1} := \alpha a_n + (1 - \alpha) b_n \qquad b_{n+1} := \frac{a_{n+1} b_n}{\beta a_{n+1} + (1 - \beta) b_n}$$

where $0<\alpha<1$ and $0<\beta<1$. In the notation of Exercise 3 of Section 8.4 this computes $G:=Q_\alpha \otimes_a (Q_\beta)_{-1}$ for $a>b$. If we let $k_n:=b_n/a_n$, we derive

$$k_{n+1}^{-1}-1=(\alpha\beta)(k_n^{-1}-1)=(\alpha\beta)^{n+1}\left(\frac{a}{b}-1\right)$$

and

$$\frac{a_n}{b_n}=1+(\alpha\beta)^n\left(\frac{a}{b}-1\right).$$

Thus

$$\frac{a_{n+1}}{a_n}=\alpha+(1-\alpha)k_n$$

and the limit is

$$G(a,b)=a\prod_{n=0}^{\infty}\left[\frac{1-\alpha(\alpha\beta)^n(1-a/b)}{1-(\alpha\beta)^n(1-a/b)}\right].$$

If we let $1-a/b=:x$ and $\alpha\beta=:q$, we have

$$G\left(1,\frac{1}{1-x}\right)=\prod_{n=0}^{\infty}\left[\frac{1-(\alpha x)q^n}{1-xq^n}\right]=\frac{\prod_{n=0}^{\infty}[1-(\alpha x)q^n]}{\prod_{n=0}^{\infty}(1-xq^n)} \tag{8.5.9}$$

which is the ratio of thetalike products occurring in the q-binomial theorem. (See Exercise 7 in Section 9.4.) Wimp [84] continues a discussion of similar calculations, all of which give linear convergence.

If we let $\alpha\beta:=\frac{1}{4}$ and $\alpha:=\frac{1}{2}$, we have a product expansion for $H_1\otimes_a H_{-1}$. Foster and Phillips [84*a*] show how this function can be closely approximated by elementary functions and can be given an elegant asymptotic expansion.

Comments and Exercises

Many other related algorithms can be found in Wimp [84]. This includes an extensive discussion of quadratically computable trigonometric integrals (in Chapter 14).

1. a) Show that $R(\alpha;\delta,\delta';x^2,y^2)=y^{-2\alpha}F(\alpha;\delta,\delta+\delta';1-x^2/y^2)$, where F is the Gaussian hypergeometric series. (See Exercise 6 in Section 1.3.)

b) Show that $R(\alpha;\delta,\delta';x^2,y^2)$ is homogeneous of degree $-\alpha$ in x^2 and y^2. Also $R(\alpha;\delta,\delta';1,1)=1$ and $R(\alpha;\delta,\delta';\cdot,\cdot)$ is continuous.

c) Verify the entries in Table 8.1.

d) Show that $[F_i,F_j]$, $i<j$, is linearly convergent for all cases except $i:=1$, $j:=2$. Observe that $[F_3,F_4]$, which is not Archimedean, has a convergence rate of 2^{-n} and $[F_2,F_3]$, which is partially comparable, has oscillatory iterates.

2. a) Observe that $C_{12}(a,b)=(\pi/2)/I(a,b)$ with

$$I(a,b):=\int_0^{\pi/2}\frac{d\theta}{\sqrt{a^2\cos^2\theta+b^2\sin^2\theta}}$$

as before.

b) Show that $C_{34}(a,b):=\sqrt{\dfrac{a^2-b^2}{2\log(a/b)}}\qquad(a\neq b).$

Hint: Use partial fractions.

c) Show that $C_{14}(a,b)$ is given by (8.4.3).
Hint: Let $(t+a^2)/(t+b^2)=:\cos^2\theta$ or $\cosh^2\theta$.

d) Show that $C_{13}(a,b)$ is given by (8.5.8) for $a<b$.

e) Use the invariance principle to verify that

$$C_{24}(b,a)=C_{32}(a,b)=\sqrt{aC_{14}(a,b)}$$

and that

$$C_{23}(b,a)=C_{42}(a,b)=\sqrt{bC_{13}(a,b)}.$$

f) This completes the analysis of all of Carlson's means in explicit form. Attempt to verify part e) directly from Theorem 8.6.

3. Use the invariance of C_{13} to show that

i) $\operatorname{arcsl} x=\sqrt{2}\operatorname{arcslh} y$
where $(1+y^4)(1+\sqrt{1-x^4})=2$, and

ii) $\operatorname{arcsl} x=2\operatorname{arcsl} z$
where $x=:2z\sqrt{1-z^4}/(1+z^4)$ and $z^2<\sqrt{2}-1$.

This is Jacobi's duplication formula for arcsl (Watson [33]).

4. Show that with $M(a,b)=G(a,H_{p/2}(a,b))=:N(b,a)$,

$$M\otimes N(a,b)=\mathcal{L}_p(a,b)=\left[\frac{a^p-b^p}{p\log(a/b)}\right]^{1/p}.$$

5. (*Carlson* [75]) Let $a,b>0$ and set

$$F(a,b):=\frac{2}{\pi}\int_0^{\pi/2}\log(a\sin^2\theta+b\cos^2\theta)\,d\theta.$$

a) Show that

$$F\left[\left(\frac{a+b}{2}\right)^2, ab\right] = 2F(a, b).$$

b) Using a) (or directly) show that

$$F(a, b) = 2 \log\left(\frac{\sqrt{a}+\sqrt{b}}{2}\right) = \log H_{1/2}(a, b).$$

6. (*Carlson* [78]) Let a, b, c, λ real be given. Assume $a+\lambda$, $b+\lambda$, $c+\lambda \geq 0$, and at most one of these is zero. Consider

$$T(\lambda) := T(a, b, c; \lambda) := \int_\lambda^\infty [(a+t)(b+t)(c+t)]^{-1/2}\, dt.$$

Let

$$k := \lambda + \sqrt{(\lambda+a)(\lambda+b)} + \sqrt{(\lambda+b)(\lambda+c)} + \sqrt{(\lambda+a)(\lambda+c)}.$$

a) Show that $T(\lambda) = 2T(k)$.
b) Show that $T(\lambda_0) = \lim_{n\to\infty} 2^{n+1} k_n^{-1/2}$, where iteratively $\lambda := k_n$, $k_{n+1} := k$, and $\lambda =: k_0$.
c) Show that for $a, b, c, d > 0$,

$$\int_0^\infty [(t+a^2)(t+b^2)(t+c^2)(t+d^2)]^{-1/2}\, dt = T(A, B, C; 0)$$

where $A := (ab+cd)^2$, $B := (ac+bd)^2$, and $C := (ad+bc)^2$.

7. (*Tricomi* [65]) Let $0 \leq k \leq 1$ be given. Set

$$R_k(a, b) := \sqrt{k^2a^2 + k'^2b^2} \qquad k' := \sqrt{1-k^2}$$

and

$$M(a, b) := \frac{a + R_k(a, b)}{b + R_k(a, b)}\, b \qquad 0 < a < b.$$

a) Show that M is a strict mean on $0 < a < b$.
b) Show that

$$M \otimes_a G(a, b) := b \prod_{n=1}^{\infty} \mathrm{cn}(2^{-n} v_0)$$

where $\mathrm{cn}(v_0) := a_0/b_0$ and $0 < v_0 < 2K$.
Hint: Use the half-angle formula for cn

$$(8.5.10) \qquad cn^2\left(\frac{1}{2}u\right) = \frac{cn(u) + \sqrt{k'^2 + k^2cn^2(u)}}{1 + \sqrt{k'^2 + k^2cn^2(u)}}$$

and deduce that $\mathrm{cn}(v_n) := a_n/b_n$ satisfies $v_{n+1} = v_n/2$ and $b_{n+1}/b_n = \sqrt{a_{n+1}/b_n} = a_{n+1}/b_{n+1} = cn(v_0/2^{n+1})$.

c) Recover Borchardt's algorithm by considering $k := 0$.

8. Compute a formula for the MacLaurin series for $G(1-x, 1)$ in (8.5.9).

8.6 *SERIES EXPANSIONS OF CERTAIN MEANS*

For homogeneous means it is particularly easy to compute Taylor series. It suffices to expand the trace around 1. In the exercises we list various series taken from Gould and Mays [84], extending results in Lehmer [71].

$$H_p(1, 1-x) = 1 - \frac{1}{2}x + \frac{p-1}{8}x^2 + \frac{p-1}{16}x^3 - \frac{(p-1)(p-3)(2p+5)}{384}x^4 + \cdots. \tag{8.6.1}$$

Similarly,

$$L_p(1, 1-x) = 1 - \frac{x}{2} + \frac{p-1}{4}x^2 + \frac{p-1}{8}x^3 - \frac{(p^2-1)(p-3)}{48}x^4 + \cdots. \tag{8.6.2}$$

From these it follows that the only means which are both Holder and Lehmer means are H_{-1}, A, and G. (See Exercise 5.) Similarly, but slightly more elaborate, analysis shows that the following theorem holds.

***Theorem 8.7** (Lehmer)*

(*a*) $$H_p \otimes_g H_q = H_s \qquad p \neq q$$

if and only if $p + q = s = 0$.

(*b*) $$L_p \otimes_g L_q = L_s \qquad p \neq q$$

if and only if $p + q = 2s = 0, 1, 2$.

(*c*) $$L_p \otimes_g L_q = H_s \qquad p \neq q$$

if and only if $p + q - 1 = s = -1, 0, 1$.

(*d*) $$H_p \otimes_g L_q = L_s \qquad p \neq q$$

if and only if $p = -q$ and $s = \frac{1}{2}$.

Proof. Sufficiency is easy in each case. Necessity is more elaborate and in some cases somewhat tedious. (See Exercise 6.) In essence it follows from the invariance principle and the computation of the first few terms of the Taylor series of the limit. □

Thus only A, G, and H can arise in such compounding. Lehmer continues by studying in detail the Taylor series of $A \otimes_g L_2$, various properties of which had been previously examined by Stieltjes in a letter to Hermite (Hermite and Stieltjes [05, letter 323]). (See Exercise 7.)

Comments and Exercises

Theorem 8.7, while very pretty, is of limited ambit, since it cannot diagnose whether the compounded mean is equivalent to a mean in the class.

1. Show that the Holder means satisfy

$$H_p(1, 1-x) = \sum_{n=0}^{\infty} A(p, n)x^n$$

where

$$A(p, n) := (-1)^n \sum_{k=0}^{n} \binom{1/p}{k} 2^{-k} \sum_{i=0}^{k} (-1)^{k-i} \binom{k}{i} \binom{pi}{n}$$

for $n \geq 1$.

2. (*Euler*) If $g(x) := \Sigma_{n=0}^{\infty} a_n x^n$ and $g^p(x) =: \Sigma_{n=0}^{\infty} b_n x^n$, then

$$\sum_{k=0}^{n} [k(p+1) - n] a_k b_{n-k} = 0 \qquad n \geq 0 .$$

3. Show that the Stolarsky means satisfy

$$S_{p+1}(1, 1-x) = \sum_{n=1}^{\infty} D(p, n)x^n$$

where

$$D(p, n) := \frac{1}{np} \sum_{k=0}^{n-1} (-1)^{n+k+1} \binom{p}{n-k} \frac{kp+k-n}{n-k+1} D(p, k) .$$

4. a) Show that the Gini means satisfy

$$G_{s,r}(1, 1-x) = \hat{G}_{r,s}(1, 1-x)\hat{G}_{s,r}(1, 1-x)$$

where

$$\hat{G}_{s,r}(a, b) := \left(\frac{a^s + b^s}{2}\right)^{1/(s-r)} .$$

b) Show that

$$\hat{G}_{s,r}(1, 1-x) := \sum_{n=0}^{\infty} \hat{G}(s, r, n)x^n$$

where

$$\hat{G}(s, r, n) = (-1)^n \sum_{k=0}^{n} \binom{1/(s-r)}{k} 2^{-k} \sum_{i=0}^{k} (-1)^{k-i} \binom{k}{i} \binom{si}{n} .$$

c) Thus $G_{s,r}$ can be computed by convolution. A similar result exists for $E_{r,s}$.

5. Show that $H_q = L_p$ if and only if $p = 0$ and $q = -1$; $p = 1$ and $q = 1$; or $p = \frac{1}{2}$ and $q = 0$.

6. Prove Theorem 8.7.

7. (*Lehmer*) Let

$$R(x) := A \otimes_g L_2(1, 1+4x) .$$

a) Show that

$$R(x) = 1 + 2 \sum_{n=0}^{\infty} \frac{x^{2^n}}{P_0 P_1 P_2 \cdots P_n}$$

where the P_i are defined recursively by $P_0(x) := 1$ and $P_{n+1}(x) := [P_n(x)]^2 + 2x^{2^n}$.
Hint: If

$$a_n := \frac{P_n}{P_1 P_2 \cdots P_{n-1}} \qquad a_0 := 1$$

$$b_n := \frac{P_{n+1} + 2x^{2^n}}{P_1 P_2 \cdots P_n} \qquad b_0 := 1 + 4x$$

$$c_n := \frac{2x^{2^n}}{P_1 P_2 \cdots P_n} \qquad c_0 := 2x$$

then

$$a_{n+1} = \frac{a_n + b_n}{2}$$

$$b_{n+1} = \frac{a_n^2 + b_n^2}{a_n + b_n}$$

$$c_{n+1} = \frac{b_{n+1} - a_{n+1}}{2} .$$

Now observe that

$$R(x) = a_0 + \sum_{i=0}^{\infty} (a_{i+1} - a_i)$$

and use the invariance principle.

b) Show independently that

$$R(x) = 1 + \sum_{n=1}^{\infty} g_n x^n$$

where $g_1 := 2$ and g_m, $m \geq 2$, satisfies the recursion

$$g_m := (-1)^m \sum_{k=1}^{\lfloor m/2 \rfloor} 2^{m-2k} \binom{m-2}{m-2k} g_k .$$

Observe that the g_i are integers.

Hint: Show that the series for R satisfies

$$R(x) = (1+2x)R\left(\frac{x^2}{(1+2x)^2}\right).$$

c) Use b) to compute g_m for $m \leq 20$. ($g_{20} = 23335660$.)

8.7 *MULTIDIMENSIONAL MEANS AND ITERATIONS*

Most of the results of this chapter have direct analogues for functions of more than two variables. Often these follow by similar arguments. We concentrate on mean iterations. Let $\bar{a} := (a_1, \ldots, a_N)$ be any strictly positive vector.

An N-dimensional *mean* is any continuous function M such that

$$\bigwedge_{i=1}^{N} a_i \leq M(\bar{a}) \leq \bigvee_{i=1}^{N} a_i \tag{8.7.1}$$

for all $a_i > 0$. The mean is *strict* if

$$\bigwedge_{i=1}^{N} a_i < \bigvee_{i=1}^{N} a_i \Rightarrow \bigwedge_{i=1}^{N} a_i < M(\bar{a}) < \bigvee_{i=1}^{N} a_i . \tag{8.7.2}$$

Also M is *symmetric* if $M(\bar{a}) = M(\bar{b})$ for any permutation $\bar{b}$ of $\bar{a}$. Homogeneity and isotonicity are defined analogously. The Lehmer and Holder means are defined by

$$L_p(\bar{a}) := \frac{\Sigma_{i=1}^{N} a_i^p}{\Sigma_{i=1}^{N} a_i^{p-1}} \tag{8.7.3}$$

and

$$H_p(\bar{a}) := \left(\frac{1}{N} \sum_{i=1}^{N} a_i^p\right)^{1/p} \tag{8.7.4}$$

respectively.

Given N N-dimensional means $M^1, \ldots, M^N$, we consider the iteration $[M^1, \ldots, M^N]$ defined by $\bar{a}_0 := \bar{a} > 0$ and

$$a_{n+1}^i := M^i(\bar{a}_n) \qquad 1 \leq i \leq N. \tag{8.7.5}$$

We write this vectorially as $\bar{a}_{n+1} := \bar{M}(\bar{a}_n)$ and denote the common limit when it exists by $\otimes_{i=1}^{N} M^i$. Again, when each M_i is symmetric, we consider this to be a *Gaussian iteration* with limit $\bigotimes_{g\, i=1}^{N} M^i$. Similarly, if

$$a_{n+1}^i := M^i(a_{n+1}^1, a_{n+1}^2, \ldots, a_{n+1}^{i-1}, a_n^i, \ldots, a_n^N) \tag{8.7.6}$$

we have an *Archimedean iteration* (there are other possible generalizations) with limit $\bigotimes_{a\, i=1}^{N} M^i$. Under mild hypotheses the convergence results of Section 8.4 remain valid.

Theorem 8.8

Let $M^1, M^2, \ldots, M^N$ be strict N-dimensional means.

(*a*) Then $\otimes_{i=1}^{N} M^i$ exists and is a strict, continuous mean.

(*b*) Suppose that the means are symmetric and continuously differentiable. Let $a_n := \bigvee_{i=1}^{N} a_n^i$ and $b_n := \bigwedge_{i=1}^{N} a_n^i$. Then, if $a_n \neq b_n$,

$$\lim_{n\to\infty} \frac{|a_{n+1} - b_{n+1}|}{|a_n - b_n|} = 0 \tag{8.7.7}$$

and convergence is superlinear in the Gaussian iteration.

(*c*) If, in fact, the means are twice continuously differentiable, convergence in the Gaussian iteration is quadratic (uniformly on compact subsets).

(*d*) Convergence is linear in the Archimedean iteration for continuously differentiable symmetric means.

Proof.

(*a*) Much as before, $a_n \geq a_{n+1} \geq b_{n+1} \geq b_n$, and we may suppose a_n converges to a and b_n converges to b. Let $\bar{c}$ be any cluster point of $\{\bar{a}_n\}$, which is bounded. Then $b \leq \bigwedge_{i=1}^{N} c_i \leq \bigvee_{i=1}^{N} c_i \leq a$, and

$$a = \bigvee_{i=1}^{N} M^i(\bar{c}) \qquad b = \bigwedge_{i=1}^{N} M^i(\bar{c}) .$$

Since all the means are strict, we must have $c_i = a$ and $c_i = b$ for each i. Thus $a = b$, and the iteration converges, say, to α. As before, the limit is a continuous strict mean.

(*b*) By symmetry we have $M^i_{,k}(ce) = 1/N$ for any i, k and any multiple of the unit vector e. Thus

$$a^i_{n+1} - \alpha = \frac{1}{N}\sum_{k=1}^{N}[(a^k_n - \alpha) + o(a^k_n - \alpha)]\,.$$

Hence

$$|a^i_{n+1} - a^j_{n+1}| = o(a^i_n - \alpha) + o(a^j_n - \alpha) = o(a_n - b_n)$$

and (8.7.7) follows.

(*c*) This is argued as in the two-variable case and relies on the fact that the Hessian $\nabla^2 M^i(\alpha, \alpha, \ldots, \alpha)$ sums to zero and has all diagonal entries equal to $-(N-1)y^i$, where each off-diagonal entry equals y^i. Thus for each i and j,

$$a^i_{n+1} - a^j_{n+1} = \frac{y^j - y^i}{2}\sum_{h<k}(a^h_n - a^k_n)^2 + o((a_n - b_n)^2)$$

(and unless all y^i coincide, convergence will be at best quadratic). Now

$$0 \le a_{n+1} - b_{n+1} \le B|a_n - b_n|^2 + o(|a_n - b_n|^2)$$

where B is an easily computable constant depending on the means, initial values, and dimension. This shows (*c*).

(*d*) We leave (*d*) as Exercise 2b). □

EXAMPLE 8.5 (SCHLÖMILCH) Consider

$$a_{n+1} := \frac{a_n + b_n + c_n}{3} \qquad =: M^1(a_n, b_n, c_n)$$

$$b_{n+1} := \sqrt{\frac{a_n b_n + b_n c_n + a_n c_n}{3}} \qquad =: M^2(a_n, b_n, c_n)$$

$$c_{n+1} := (a_n b_n c_n)^{1/3} \qquad =: M^3(a_n, b_n, c_n)\,.$$

This is a quadratically convergent Gaussian iteration, as follows from Theorem 8.8(*c*). (Since $M^1 \ge M^2 \ge M^3$, M^2 is a strict mean.) Let $S(a, b, c)$ denote the limit. While we cannot identify S, we can, following Landau, observe that if $ac = b^2$, then $a_n c_n = b_n^2$ and thus

$$S(a, \sqrt{ac}, c) = \mathrm{He} \otimes_g G(a, c) =: S(a, c) \tag{8.7.8}$$

where $\mathrm{He}(a, c) := (a + \sqrt{ac} + c)/3 = E_{3/2,1/2}(a, c)$ is the Heronian mean. While this does not appear to have a closed form, it has an attractive product expansion,

$$S(1, x) = \prod_{n=0}^{\infty} \frac{1 + \sqrt{x_n} + x_n}{3} \tag{8.7.9}$$

where $x_0 := x$ and

$$x_{n+1} := \frac{3\sqrt{x_n}}{1 + \sqrt{x_n} + x_n}\,.$$

While it is difficult to evaluate two-dimensional compound means, it appears even harder to evaluate higher dimensional ones.

There is a satisfactory analogue of Proposition 8.3. Let f be continuous and strictly monotone as before. Let $a_0, a_1, \ldots, a_N$ be distinct positive real numbers. Let $F_{(N)}$ be any Nth antiderivative for f. We define

$$M_{\int_{N^f}}(a_0, a_1, \ldots, a_n) := f^{-1}\left[N!\sum_{k=0}^{N}\frac{F_{(N)}(a_k)}{\Pi_{k\ne j}(a_k - a_j)}\right]. \tag{8.7.10}$$

Then $M_{\int_{N^f}}$ is a strict, symmetric N-dimensional mean. (See Exercise 5.)

We should emphasize that the invariance principle continues to hold: $\Phi := \otimes_{i=1}^{N} M^i$ is the unique continuous diagonal mapping satisfying

$$\Phi = \Phi(M^1, M^2, \ldots, M^N)\,. \tag{8.7.11}$$

Comments and Exercises

A wealth of information on N-dimensional means can be found in Hardy, Littlewood, and Polya [59]. The Lehmer means are studied in Beckenbach [50]. The Schlömilch mean and Landau's contribution are discussed in Schoenberg [77]. Various N-dimensional quadratic iterations are exhibited in Wimp [84] and Arazy et al. [Pr].

1. a) Show that H_p and L_p are strict, homogeneous, symmetric means.
   b) Show that $(\Pi_{i=1}^{N} a_i)^{1/N} = \lim_{p\to 0} H_p(\bar a) =: H_0(\bar a)$.
   c) Show that H_p is convex for $p \ge 1$ and that L_p is convex for $1 \le p \le 2$.

2. a) Show that $\otimes_{i=1}^{N} M^i$ is a continuous strict mean when each M^i is.
   b) Show that convergence is linear in the Archimedean iteration.
   c) Estimate the rate in the three-variable case.
   d) Show that

$$\bigotimes_{i=1}^{N}{}_a H_p(\bar{a}) = \left[\frac{2}{N(N+1)} \sum_{k=1}^{N} k a_k^p\right]^{1/p} \qquad p \neq 0$$

and

$$\bigotimes_{i=1}^{N}{}_a H_0(\bar{a}) = \left[\prod_{k=1}^{N} a_k^k\right]^{2/N(N+1)}.$$

Hint: Use the invariance principle when $p := 1$.

3. Show that $S(1, x)$ satisfies (8.7.9). Compare this to the product expansion for $\mathscr{L}(1, x)$.

4. a) Let

$$M^1(a, b, c) := \frac{a+b+c}{3}$$

$$M^2(a, b, c) := \frac{ab+bc+ac}{a+b+c}$$

and

$$M^3(a, b, c) := \frac{3abc}{ac+ab+bc} = \frac{3}{1/a+1/b+1/c}.$$

Show that

$$\bigotimes_{i=1}^{3}{}_g M^i(a, b, c) = (abc)^{1/3}$$

and that convergence is quadratic.

b) Let S_k be the kth *elementary symmetric mean function* of N variables. That is, $S_k := f_k/\binom{N}{k}$ with f_k as in Exercise 6 of Section 11.2. Thus, $S_0 := 1$, $S_1 := H_1$, etc. Let $M^k := S_k/S_{k-1}$ for $1 \leq k \leq n$. Show that $M^k \geq M^{k+1}$ and that $\bigotimes_{i=1}^{N}{}_g M^i = H_0$.

c) In a) replace M^2 by H_0. Thus

$$a_{n+1} := \frac{a_n+b_n+c_n}{3} \qquad b_{n+1} := (a_n b_n c_n)^{1/3}$$

$$c_{n+1} := \frac{3}{1/a_n+1/b_n+1/c_n}.$$

Show that the limit mean M satisfies

$$M(a, \sqrt{ac}, c) = \mathrm{He} \otimes_g \mathrm{He}_{-1}(a, c) = \sqrt{ac} = (abc)^{1/3}.$$

This is not the general limit.

d) More generally, whenever M is homogeneous and symmetric, $\Phi = M \otimes G \otimes M_{-1}$ satisfies $\Phi(a, \sqrt{ac}, c) = \sqrt{ac}$. Similar results hold in N dimensions.

5. a) Show that $M_{\int_N f}$ of (8.7.10) is uniquely defined and is a strict mean. *Hint*: Let

$$P_N(x) := \sum_{k=0}^{N} F_{(N)}(a_k) \frac{\Pi_{j\neq k}(x-a_j)}{\Pi_{j\neq k}(a_k-a_j)}.$$

Then P_N is the Lagrange interpolating polynomial for $F_{(N)}$ at $a_0, a_1, \ldots, a_N$. (See Exercise 1 of Section 10.1.) Thus $P_N^{(N)}$ and f must agree at some point strictly between $\bigwedge_{i=1}^{N} a_i$ and $\bigvee_{i=1}^{N} a_i$. Now show that $M_{\int_N f}$ extends continuously to all strictly positive variables. The harder part is to show it is strict.

b) Show that the three-dimensional Stolarsky means are appropriately defined (and are homogeneous) if

$$S_p(a, b, c) := \left[\frac{2}{p(p-1)}\left(\frac{a^p}{(a-b)(a-c)} + \frac{b^p}{(b-a)(b-c)} + \frac{c^p}{(c-a)(c-b)}\right)\right]^{1/(p-2)}$$

for $p \neq 0, 1, 2$. Also

$$S_0(a, b, c) := \left[\frac{(a-b)(b-c)(c-a)}{2(b-c)\log a + 2(c-a)\log b + 2(a-b)\log c}\right]^{1/2}$$

while

$$S_1(a, b, c) := \frac{(a-b)(b-c)(a-c)}{2(b-c)a\log a + 2(c-a)b\log b + 2(a-b)c\log c}$$

and, using $f(x) := \log$, that the identric mean may be given as

$$\mathscr{I}(a, b, c) := S_2(a, b, c) := \exp\left[\frac{a^2\log a}{(a-b)(a-c)} + \frac{b^2\log b}{(b-a)(b-c)} + \frac{c^2\log c}{(c-a)(c-b)} - \frac{3}{2}\right].$$

c) Show that the N-dimensional logarithmic mean is given by

$$\mathscr{L}_N(a_1, a_2, \ldots, a_N) := \left[(-1)^N(N-1)\sum_{i=1}^{N} \frac{\log a_i}{\Pi_{j\neq i}(a_i-a_j)}\right]^{-1/(N-1)}$$

d) Investigate the isotonicity of $S_p(a, b, c)$ as a function of p.

6. There are various multidimensional generalizations of the AGM due to Borchardt [1888] and others. In four variables one may take

$$a_{n+1} := \frac{a_n + b_n + c_n + d_n}{4}$$

$$b_{n+1} := \frac{\sqrt{a_n b_n} + \sqrt{c_n d_n}}{2}$$

$$c_{n+1} := \frac{\sqrt{a_n c_n} + \sqrt{b_n d_n}}{2}$$

$$d_{n+1} := \frac{\sqrt{a_n d_n} + \sqrt{b_n c_n}}{2} .$$

a) Observe that, while the means are not all symmetric, the derivatives on the diagonal ($a = b = c = d$) all coincide, and hence establish quadratic convergence.

b) Show that when $a_0 := b_0$ and $c_0 := d_0$, the iteration reduces to the AGM. This iteration shares many of AGM's attributes (Arazy et al. [Pr]).

7. (*An extended convergence result*)

a) Observe that Theorem 8.8 continues to hold if the condition that the means are strict is relaxed to

$$\overline{M}(\bar{c}) = \bigvee_{i=1}^{N} c_i \quad \text{and} \quad \underline{M}(\bar{c}) = \bigwedge_{i=1}^{N} c_i \quad \text{implies} \quad \bigwedge_{i=1}^{N} c_i = \bigvee_{i=1}^{N} c_i .$$

Here

$$\underline{M} := \bigwedge_{i=1}^{N} M^i \quad \text{and} \quad \bar{M} := \bigvee_{i=1}^{N} M^i .$$

This clearly holds if $N-1$ of the means are strict.

b) More interestingly, use a) to establish the following result. Let A be an entry-positive N by N matrix. Set $\mathrm{A}_0 := \mathrm{A}$ and

$$\mathrm{A}_{n+1} := \frac{1}{N}\left({}^*\sqrt{\mathrm{A}_n}\right)^2$$

for $n \geq 0$. Here ${}^*\sqrt{\cdot}$ represents entrywise square root. Then A_n converges to a constant matrix with entry $e(\mathrm{A})$.

c) If $\mathrm{A} := \begin{pmatrix} a & b \\ b & a \end{pmatrix}$ then $e(\mathrm{A}) = \mathrm{AG}(a, b)$.

d) If $\mathrm{A} := \begin{pmatrix} a & a \\ b & b \end{pmatrix}$ then $e(\mathrm{A}) = \mathscr{L}(a, b)$.

e) Similarly consider A_0 and B_0 entry positive and

$$\mathrm{A}_{n+1} := \frac{\mathrm{A}_n + \mathrm{B}_n}{2} \qquad \mathrm{B}_{n+1} := \frac{1}{N}\, {}^*\sqrt{\mathrm{A}_n \mathrm{B}_n} .$$

Show that this iteration converges to a constant matrix. (See Cohen and Nussbaum [Pr].)

8.8 *ALGEBRAIC ITERATIONS AND FUNCTIONAL RELATIONS*

Among the more familiar and fundamental properties of the exponential function is that it satisfies the algebraic functional relation

$$f(z) = [f(z/n)]^n . \tag{8.8.1}$$

Are there any other algebraic functional relations of the form

$$f(z) = \beta(f(\mu(z), z)) \tag{8.8.2}$$

where β and μ are algebraic? More precisely, μ is an *algebraic function* if there exists a polynomial P in two variables with coefficients in some base field F (for most of this discussion $F := \mathbb{Q}$ or $F := \mathbb{C}$) such that

$$P(\mu(z), z) = 0 \tag{8.8.3}$$

and Ω is an algebraic functional relation for f if Ω is a polynomial in three variables over F and there exists an algebraic function μ so that

$$\Omega(f(z), f(\mu(z)), z) = 0 . \tag{8.8.4}$$

The function μ is termed an *algebraic transformation* (for f). We assume throughout that z is a complex variable and unless otherwise indicated that f is defined on a region U which contains an open set V so that $\mu(V) \subset U$. [This ensures that (8.8.4) can be continued to any open connected component of the domain of f that contains U.] The collection of all such transformations satisfying (8.8.4) for some Ω we denote by $\mathrm{TG}(f : F)$, the *algebraic transformation group* of f over F. If

$$L(x) := M \otimes N(1, x) \tag{8.8.5}$$

where M and N are homogeneous means, then

$$L(x) = M(x) L(\mu(x)) \tag{8.8.6}$$

where $M(x) := M(1, x)$ and $\mu(x) := N(1, x)/M(1, x)$. Thus if both M and N are algebraic, then L satisfies an algebraic functional relation with algebraic transform μ. It transpires that the transformation groups of the most elementary transcendental functions are very simple, too simple in fact, to support quadratically converging mean iterations. (See Exercise 1.) This, in part, explains why the algorithms of Chapter 7 for exp and log require the intermediate use of nonelementary transcendental functions.

We wish now to compute the algebraic transformation groups of some familiar functions. However, we need first to establish the transcendence [over $\mathbb{C}(z)$] of the functions exp, log, and exp(exp). This is considerably easier than the arguments for the transcendence of numbers such as e. The arguments are roughly the same for all the above functions. For exp it proceeds as follows. Suppose exp satisfies an equation of the form

$$\sum_{i=0}^{k} a_i \exp(iz) = 0 \tag{8.8.7}$$

where the a_i are rational functions, k is assumed minimal, and $a_0 = 1$. We differentiate (8.8.7) to get

$$\sum_{i=1}^{k} (\dot{a}_i + ia_i) \exp(iz) = 0\,. \tag{8.8.8}$$

If $k \geq 2$ and we divide (8.8.8) by $\exp(z)$, we obtain a lower order expression than (8.8.7) and violate the minimality of k. To dispose of the $k = 1$ case we must show that exp is not a rational function. Since exp is entire, if it were rational it would in fact have to be polynomial, and if it were polynomial it would have to have a finite Taylor expansion.

Theorem 8.9

(*a*) $\mathrm{TG}(\exp: \mathbb{Q}) = \{az: a \text{ rational}\}$
(*b*) $\mathrm{TG}(\log: \mathbb{Q}) = \{z^b: b \text{ rational}\}$
(*c*) $\mathrm{TG}(\exp(\exp): \mathbb{Q}) = \{z\}$.

Proof. We will prove, by elementary methods, that

(a') $\mathrm{TG}(\exp: \mathbb{Q}) = \{az + b: a \text{ rational}, \exp(b) \text{ and } b \text{ algebraic}\}$
(b') $\mathrm{TG}(\log: \mathbb{Q}) = \{az^b: \log(a) \text{ and } a \text{ algebraic}, b \text{ rational}\}$
(c') $\mathrm{TG}(\exp(\exp): \mathbb{Q}) = \{z + b: \exp(b) \text{ and } b \text{ algebraic}\}$.

To see that (a), (b), (c) and (a'), (b'), (c') are the same is equivalent to Lindemann's theorem which guarantees that $\exp(a)$ is transcendental for any algebraic $a \neq 0$. (See Exercise 7 of Section 11.2.)

We first prove part (a'). Suppose that μ is an algebraic transformation for exp. Then there exists an expression of the form

$$\sum_{i=0}^{k} a_i \exp(m_i z) \exp(n_i \mu(z)) = 0 \tag{8.8.9}$$

where the a_i are nonzero algebraic functions in z and the m_i and n_i are integers. Equivalently,

$$\sum_{i=0}^{k} a_i \exp(m_i z + n_i \mu(z)) = 0 \tag{8.8.10}$$

where we assume k is minmal, that is, we assume (8.8.10) contains a minimum number of distinct nonzero $\exp(m_i z + n_i \mu(z))$ terms. If we divide (8.8.10) by its last term and differentiate, we get

$$\sum_{i=0}^{k-1} \left\{[m_i - m_k + (n_i - n_k)\dot{\mu}]\left(\frac{a_i}{a_k}\right) + \left(\frac{a_i}{a_k}\right)^{\cdot}\right\} \exp[(m_i - m_k)z + (n_i - n_k)\mu] = 0 \tag{8.8.11}$$

This expression has one less term than (8.8.10) and contradicts the minimality of (8.8.10) unless (8.8.11) contains no nonzero terms. This implies that each term of (8.8.10) must be constant. Thus there exist m and n integral and a nonzero algebraic function $a(z)$ so that

$$a(z) \exp(mz + n\mu(z)) = \text{constant}\,. \tag{8.8.12}$$

Since exp is transcendental, $mz + n\mu(z)$ must be constant. Call this constant b; since μ is algebraic over $\mathbb{Q}$, b must be algebraic. Specializing (8.8.12) at $z = 0$ shows that $\exp(b)$ must also be algebraic. Part (a') is completed by observing that $\mu(z) = (m/n)z + b$ is an algebraic transform of exp.

The proof of part (b') is similar. If μ is an algebraic transform for log, then there exists an expression of the form

$$\sum_{i=0}^{k} a_i [\log(z)]^{m_i} \cdot [\log(\mu(z))]^{n_i} = 0 \tag{8.8.13}$$

where the a_i are algebraic functions and the m_i and n_i are nonnegative integers. Let (8.8.13) be minimal in the sense that it has the smallest maximal degree and contains the fewest distinct terms of maximal degree. (The degree of a term is $m_i + n_i$.) Suppose the term corresonding to $i = 0$ is such a maximal term. If we now divide (8.8.13) by a_0 and differentiate, we are left with an expression containing fewer maximal terms, which contradicts minimality unless all the transcendental terms vanish under differentiation. In particular (8.8.13) must actually be of the form

$$b \log(z) + c \log(\mu(z)) = d \tag{8.8.14}$$

where b, c, and d are algebraic numbers. Thus

(8.8.15) $$\mu(z) = \exp(d/c) z^{-b/c}$$

and we see that μ is algebraic exactly when $\exp(d/c)$ is algebraic and $-b/c$ is rational. (Otherwise, by Exercise 2, $z^{-b/c}$ is transcendental.) This finishes (b').

The proof of (c') is again similar to (a'). There are, however, a few additional wrinkles. Suppose now that $\mu(z)$ is an algebraic transform for $\exp(\exp(z))$. Consider minimal length sums of the form

(8.8.16) $$\sum_{i=0}^{k} a_i \exp[m_i \exp(z) - n_i \exp(\mu(z))] = 0$$

where the a_i are algebraic functions of z, $\exp(z)$, and $\exp(\mu(z))$. Dividing and differentiating (8.8.16) leads, as in (a'), to a contradiciton unless

(8.8.17) $$m_i \exp(z) - n_i \exp(\mu(z)) = \text{constant}$$

and the result follows. One of the wrinkles is that we must establish the transcendence of $\exp(\exp(z))$ over the algebraic functions in z, $\exp(z)$, and $\exp(\mu(z))$. This is necessary for our minimality argument and can be done analogously to proving that exp is transcendental. (See Exercise 2.) □

The transformations we are considering are algebraic over $\mathbb{Q}$. This is a natural choice for computationally related questions. The analogous results for algebraic transformations over $\mathbb{C}$ are similar but easier because the number theoretic details vanish. We have the following:

Theorem 8.10

(*a*) $\text{TG}(\exp: \mathbb{C}) = \{az + b: a \in \mathbb{Q} \text{ and } b \in \mathbb{C}\}$.
(*b*) $\text{TG}(\log: \mathbb{C}) = \{az^b: b \in \mathbb{Q} \text{ and } a \in \mathbb{C}\}$.
(*c*) $\text{TG}(\exp(\exp): \mathbb{C}) = \{z + b: \exp(b) \in \mathbb{Q}\}$.

If $f(z) = g(a(z))$, where $a(z)$ is an algebraic function, then

(8.8.18) $$\text{TG}(g: F) = a \circ \text{TG}(f: F) \circ a^{-1}.$$

EXAMPLE 8.6 Let μ be an algebraic function and suppose $\mu^{(n)}$ is the identity. [For example, $\mu(z) := rz$, where r is an nth root of unity.] Then

(8.8.19) $$f := \exp(\mu^{(1)}) + \exp(\mu^{(2)}) + \cdots + \exp(\mu^{(n)})$$

is invariant under μ, where $\mu^{(n)} := \mu(\mu^{(n-1)})$. Note that $\text{TG}(f)$ is not in general conjugate to TG(exp) since TG(exp) contains no finite elements of order greater than 2.

For q^z and $\log_q(z)$, where q is an algebraic number distinct from 0 and 1 we have

(8.8.20) $$\text{TG}(q^z : \mathbb{Q}) = \{az + b: a \text{ and } b \text{ rational}\}$$

and

(8.8.21) $$\text{TG}(\log_q : \mathbb{Q}) = \{az^b: a \text{ and } b \text{ rational}\}.$$

To derive these results we first observe that (a') and (b') of Theorem 8.9 hold for the above functions (with exp replaced by q^z and log replaced by $\log_q$). The only difficult part is to show that q^a and a are simultaneously algebraic exactly when a is rational. This is the celebrated Gelfond-Schneider theorem. (See Section 11.2.)

In Exercises 1 and 5 we show that functions like $\beta(e^{\gamma(z)}, z)$ and $\beta(\log \gamma(z), z)$, where $\beta(\cdot,\cdot)$ and $\gamma(\cdot)$ are algebraic, cannot support functional equations that possess quadratic fixed points in their domain of analyticity. In particular such functions cannot be the limit of quadratically convergent homogeneous mean iterations. This shows why the elementary functions are always associated with linearly convergent iterations.

Comments and Exercises

The results of the section underscore the difficulties of analyzing in closed form the limits of mean iterations. The familiar elementary transcendental functions can only be limits of fairly trivial iterations. The arguments are extended in the exercises to cover sin, tan, arccos, and so on. Exercise 6 treats the special case of compounding rational means and shows that the limit of such a mean iteration is either the kth root of a rational function or is transcendental.

1. a) Suppose that

$$L(x) = M \otimes N(1, x)$$

as in (8.8.5), where $M(1, x)$ and $N(1, x)$ are algebraic functions analytic in a neighbourhood of 1. Show that if L can be quadratically computed by iterating (8.8.6), then μ has a fixed point at 1 of the form $\mu(x) := 1 + O(1-x)^2$ as $x \to 1$.

b) Call an algebraic transformation μ *quadratically attractive* at c if $\mu(c) = c + O(c-z)^2$ as $z \to c$. Suppose that λ is algebraically conjugate to μ. That is,

$$\lambda = \alpha \circ \mu \circ \alpha^{-1}$$

where α is algebraic. Show that λ is also quadratically attractive at c.

c) Show that none of exp, log, or exp (exp) nor any function algebraically conjugate to the above functions is the limit of a quadratically converging algebraic homogeneous mean iteration.

2. a) Prove that z^α (α irrational), log, and sin are transcendental functions over $\mathbb{C}(z)$.
b) Show that exp (exp) is transcendental over $\mathbb{C}(z, \exp(z), \exp(\mu(z)))$ when μ is algebraic.

3. Prove (8.8.20) and (8.8.21) assuming the Gelfond–Schneider theorem.

4. (*On the algebraic transformations of sin, cos, and exponential sums*) Let $\alpha(z)$ be an algebraic function over $F := \mathbb{C}(z, e^z)$, the field of rational functions in z and e^z. Suppose that $\alpha(z)$ is *not* algebraic over $\mathbb{C}(z)$. Show that

$$\mathrm{TG}(\alpha : F) \subset \{az + b : a, b \in \mathbb{C}\}$$

and calculate $\mathrm{TG}(\cos : \mathbb{C})$ and $\mathrm{TG}(\sin : \mathbb{C})$. *Outline*:

a) Show that if $\mu \in \mathrm{TG}(\alpha : \mathbb{C})$, then there exists a nontrivial relation

$$\sum_{j=0}^{d} b_j(z) \exp[k_j \mu(z) + h_j z] \equiv 0$$

with $b_j \in \mathbb{C}(z)$ and $k_j, h_j \in \mathbb{Z}$.

b) Consider minimal (in d) expressions of the above type and argue, as in the proof of the transcendence of exp, that for some j, $\exp[k_j \mu(z) + h_j z] \in \mathbb{C}(z)$.

5. a) Suppose that $\alpha(z)$ is algebraic over $\mathbb{C}(z, e^{g(z)})$ where $g(z)$ is algebraic over $\mathbb{C}(z)$, and suppose that $\alpha(z)$ is not algebraic over $\mathbb{C}(z)$. Extend the arguments of Exercises 4 and 1 to show that $\mathrm{TG}(\alpha, \mathbb{C})$ contains no elements that are quadratic at any point where g is analytic. In particular, such a function cannot be the limit of a quadratically converging algebraic homogeneous mean iteration.
b) Suppose that $\alpha(z)$ is algebraic over $\mathbb{C}(z, \log(g(z)))$ where $g(z)$ is algebraic over $\mathbb{C}(z)$ and suppose that $\alpha(z)$ is not algebraic over $\mathbb{C}(z)$. Show that $\mathrm{TG}(\alpha : \mathbb{C})$ contains no elements that are quadratic at any point where g is analytic and nonzero.

6. (*On the iteration of rational means*)

a) Let M and N be homogeneous rational means. (A rational mean is a mean that is a rational function.) Show that $M \otimes N(1, x)$ is convergent in some neighbourhood of 1. Show that either

1) $M \otimes N(1, x)$ is transcendental
or
2) $[M \otimes N(1, x)]^i$ is a rational function for some integer i.

Outline: Suppose $f(x, y) = M \otimes N(x, y)$ and suppose that $f(1, x)$ is algebraic. Then one has a finite sum

$$\sum s_i(x)[f(1, x)]^i = 0, \qquad s_i \in \mathbb{C}(x)$$

and

$$\sum r_i(x, y)[f(x, y)]^i = 0 \tag{8.8.22}$$

where $r_i(x, y) = x^{-i} s_i(y/x)$. Thus, on substituting,

$$\sum r_i(M, N)[f(M, N)]^i = 0 \tag{8.8.23}$$

while by invariance,

$$\sum r_i(x, y)[f(M, N)]^i = 0\,. \tag{8.8.24}$$

Consider a minimal expression of type (8.8.22) and deduce from (8.8.23) and (8.8.24) that, for some i,

$$\frac{r_i(M, N)}{r_0(M, N)} = \frac{r_i(x, y)}{r_0(x, y)}\,.$$

Observe that

$$\lambda^i r_i(x, y) = r_i\left(\frac{x}{\lambda}, \frac{y}{\lambda}\right)$$

and deduce by passing to the limit that

$$f(x, y) = \left[\frac{r_i(1, 1)}{r_0(1, 1)} \frac{r_0(x, y)}{r_i(x, y)}\right]^{1/i}.$$

b) Let

$$N(x, y) := \left(1 - \frac{1}{k}\right)x + \frac{1}{k}\, y$$

and

$$M(x, y) := \frac{x^{k-1} y}{M(x, y)^{k-1}}\,.$$

As in Exercise 9 of Section 8.4,

$$N \otimes M(a, b) = (a^{k-1} b)^{1/k}$$

and the convergence is quadratic. In particular case 2) of a) can occur.

c) Show that $A \otimes_g L_2(1, x)$ is transcendental. Thus case 1) of a) can also occur. (See Exercise 7 of Section 8.6.)

7. Calculate

$$\mathrm{TG}(\sin^{-1}:\mathbb{C}) \quad \text{and} \quad \mathrm{TG}(\cos^{-1}:\mathbb{C}).$$

Hint:

$$\sin^{-1} z = -i \log(iz + \sqrt{1-z^2}).$$

Chapter Nine

Some Additional Applications

Abstract. *In Section 9.1 we derive the classical formula for $r_2(n)$ and its theta function equivalent. In Sections 9.2 and 9.3 we consider the summation of various multidimensional series. Results include an alternating series test in several dimensions, evaluation of various lattice sums, and related invariants. Section 9.4 gives Watson's quintuple-product identity, and Ramanujan's ${}_1\Psi_1$ product. Section 9.5 considers quintic and septic multipliers and solvable iterations.*

9.1 *SUMS OF TWO SQUARES*

We need the following simple lemma on Lambert series whose proof (Exercise 1) proceeds by expanding both sides of each equation.

Lemma 9.1

If $|q|<1$ and $u_n := q^n/(1-q^n)$, then

$$\sum_{m=1}^{\infty} u_m(1+u_m) = \sum_{n=1}^{\infty} nu_n \tag{9.1.1}$$

and

$$\sum_{m=1}^{\infty} (-1)^{m+1} u_{2m}(1+u_{2m}) = \sum_{n=1}^{\infty} (2n-1)u_{4n-2}. \tag{9.1.2}$$

Our development hinges on yet another remarkable identity due to Ramanujan [62]. (See also Hardy and Wright [60].)

Proposition 9.1

Let θ be real with $0<\theta<\pi$. Let

$$(9.1.3)\qquad T := T(q,\theta) := \frac{1}{4}\cot\left(\frac{\theta}{2}\right) + \sum_{n=1}^{\infty} u_n \sin(n\theta)$$

$$(9.1.4)\qquad T_1 := T_1(q,\theta) := \left[\frac{1}{4}\cot\left(\frac{\theta}{2}\right)\right]^2 + \sum_{n=1}^{\infty} u_n(1+u_n)\cos(n\theta)$$

$$(9.1.5)\qquad T_2 := T_2(q,\theta) = \frac{1}{2}\sum_{n=1}^{\infty} nu_n[1-\cos(n\theta)] .$$

Then

$$T_1 + T_2 = T^2 .$$

Proof.

$$T^2 = \left[\frac{1}{4}\cot\left(\frac{\theta}{2}\right)\right]^2 + S_1 + S_2$$

where

$$S_1 := \frac{1}{2}\sum_{n=1}^{\infty} u_n \cot\left(\frac{\theta}{2}\right)\sin(n\theta)$$

and

$$S_2 := \sum_{m,n=1}^{\infty} u_m u_n \sin(m\theta)\sin(n\theta) .$$

Now

$$\frac{1}{2}\cot\left(\frac{\theta}{2}\right)\sin(n\theta) = \frac{1}{2} + \sum_{k=1}^{n-1}\cos(k\theta) + \frac{1}{2}\cos(n\theta)$$

while

$$2\sin(m\theta)\sin(n\theta) = \cos[(m-n)\theta] - \cos[(m+n)\theta] .$$

Thus

$$T^2 = \left[\frac{1}{4}\cot\left(\frac{\theta}{2}\right)\right]^2 + \sum_{k=0}^{\infty} a_k\cos(k\theta)$$

for constants $a_k(q)$ which we proceed to evaluate. Now

$$a_0 = \frac{1}{2}\sum_{n=1}^{\infty} u_n + \frac{1}{2}\sum_{n=1}^{\infty} u_n^2$$

where the $\frac{1}{2}u_n^2$ term comes from $m=n$ in S_2. Thus

$$(9.1.6)\qquad a_0 = \frac{1}{2}\sum_{n=1}^{\infty} u_n(1+u_n) = \frac{1}{2}\sum_{n=1}^{\infty} nu_n$$

by (9.11). For $k\geq 1$, S_1 contributes to a_k,

$$\frac{1}{2}u_k + \sum_{i=1}^{\infty} u_{k+i}$$

and S_2 donates

$$\frac{1}{2}\sum_{m-n=k} u_m u_n + \frac{1}{2}\sum_{n-m=k} u_m u_n - \frac{1}{2}\sum_{m+n=k} u_m u_n$$

for $m, n\geq 1$. Thus

$$a_k = \frac{1}{2}u_k + \sum_{i=1}^{\infty} u_{k+i} + \sum_{i=1}^{\infty} u_i u_{k+i} - \frac{1}{2}\sum_{i=1}^{k-1} u_i u_{k-i} .$$

Luckily,

$$u_i u_{k-i} = u_k(1+u_i+u_{k-i})$$

and

$$u_{k+i} + u_i u_{k+i} = u_k(u_i - u_{k+i}) .$$

Hence

$$(9.1.7)\qquad a_k = u_k\left[\frac{1}{2} + \sum_{i=1}^{\infty}(u_i - u_{k+i}) - \frac{1}{2}\sum_{i=1}^{k-1}(1+u_i+u_{k-i})\right]$$
$$= u_k\left(1 + u_k - \frac{1}{2}k\right) .$$

This shows that

$$T^2 = \left[\frac{1}{4}\cot\left(\frac{\theta}{2}\right)\right]^2 + \sum_{k=1}^{\infty} u_k(1+u_k)\cos(k\theta) + \frac{1}{2}\sum_{k=1}^{\infty} ku_k[1-\cos(k\theta)]$$

(9.1.8)

which is the desired result. □

For $\theta := \pi/2$ this result becomes

$$\left[1+4\sum_{n=0}^{\infty}(-1)^n\frac{q^{2n+1}}{1-q^{2n+1}}\right]^2 = 1+16\sum_{n=1}^{\infty}(-1)^n u_{2n}(1+u_{2n})$$
$$+8\sum_{n=0}^{\infty}(2n+1)(u_{2n+1}+4u_{4n+2})$$
$$=1+8\sum_{n=0}^{\infty}(2n+1)u_{2n+1}$$
$$+8\sum_{n=0}^{\infty}(4n+2)u_{4n+2}$$

on applying (9.1.2). Thus

$$\left[1+4\sum_{n=0}^{\infty}(-1)^n\frac{q^{2n+1}}{1-q^{2n+1}}\right]^2 = 1+8\sum_{\substack{n=1\\ n\not\equiv 0 \pmod 4}}^{\infty}\frac{n\cdot q^n}{1-q^n}.$$

Now (3.2.23) can be used to show that the right-hand side is $\theta_3^4(q)$. Thus

(9.1.9)
$$\theta_3^2 = 1+4\sum_{n=0}^{\infty}(-1)^n\frac{q^{2n+1}}{1-q^{2n+1}}$$
$$=1+4\sum_{n=0}^{\infty}\left[\frac{q^{4n+1}}{1-q^{4n+1}}-\frac{q^{4n+3}}{1-q^{4n+3}}\right]$$

and this last expression is nonnegative for real q. (Hardy and Wright [60] use Proposition 9.1 to deduce the formula for θ_3^4 from that for θ_3^2).

For $r=1$ or 3 let $d_r(k)$ denote the number of divisors of k congruent to r modulo 4. Then

$$\sum_{n=0}^{\infty}\frac{q^{4n+r}}{1-q^{4n+r}} = \sum_{n=0}^{\infty}\sum_{d=1}^{\infty}q^{(4n+r)d} = \sum_{k=1}^{\infty}d_r(k)q^k$$

and a comparison of the coefficients in (9.1.9) shows that

(9.1.10)
$$r_2(k) = 4[d_1(k)-d_3(k)].$$

In other words, the number of representations of a positive integer k as a sum of two squares, counting order and sign, is 4 times the surplus of divisors of k congruent to 1 modulo 4 over those congruent to 3 modulo 4.

This recovers Jacobi's classical result, a result also known to Gauss. (See Dickson [71].) Since

$$\sum_{m=1}^{\infty}\frac{q^m}{1+q^{2m}} = \sum_{m=0}^{\infty}\frac{(-1)^m q^{2m+1}}{1-q^{2m+1}}$$

we also have

(9.1.11)
$$\theta_3^2(\theta) = 1+4\sum_{m=1}^{\infty}\frac{q^m}{1+q^{2m}}.$$

This is the formula exploited in Section 3.7. Also (9.1.9) shows that

(9.1.12)
$$\theta_3^2(q) = 1+4\sum_{\substack{n,m=1\\ n\text{ odd}}}^{\infty}(-1)^{(n-1)/2}q^{nm}$$

and

(9.1.13)
$$\theta_4^2(q) = 1+4\sum_{\substack{n,m=1\\ n\text{ odd}}}^{\infty}(-1)^{(n-1)/2+m}q^{nm}$$
$$=1+4\sum_{n,m=1}^{\infty}(-1)^{n+m-1}q^{m(2n-1)}.$$

An alternative recent derivation of (9.1.9), due to Hirschhorn [85], relies only on the triple-product identity. Begin with (3.1.13) and let $a^2 := w$. This gives

$$(a-a^{-1})\prod_{n=1}^{\infty}(1-a^2q^n)(1-a^{-2}q^n)(1-q^n)$$
$$=\sum_{n=-\infty}^{\infty}a^{4n+1}q^{2n^2+n}-\sum_{n=-\infty}^{\infty}a^{4n-1}q^{2n^2-n}.$$

Now apply the triple product in form (3.1.1) to each of these sums. This leads to

(9.1.14)
$$(a-a^{-1})\prod_{n=1}^{\infty}(1-a^2q^n)(1-a^{-2}q^n)(1-q^n)$$
$$=a\prod_{n=1}^{\infty}(1+a^4q^{4n-1})(1+a^{-4}q^{4n-3})(1-q^{4n})$$
$$-a^{-1}\prod_{n=1}^{\infty}(1+a^4q^{4n-3})(1+a^{-4}q^{4n-1})(1-q^{4n}).$$

Next differentiate each side with respect to a, at 1. (Use logarithmic differentiation on each product separately.) This, after rearrangement, produces

$$1+4\sum_{n=1}^{\infty}\frac{(-1)^n q^{2n-1}}{1+q^{2n-1}}=\frac{\Pi_{n=1}^{\infty}(1-q^n)^3}{\Pi_{n=1}^{\infty}(1+q^{4n-1})(1+q^{4n-3})(1-q^{4n})}.$$

(9.1.15)

The right-hand side of (9.1.15) is

$$\frac{\Pi_{n=1}^{\infty}(1-q^n)^3}{\Pi_{n=1}^{\infty}(1+q^n)(1-q^{2n})}=\frac{\Pi_{n=1}^{\infty}(1-q^n)^2}{\Pi_{n=1}^{\infty}(1+q^n)^2}=\theta_4^2(q)$$

where the last equality follows from (3.1.4) and (3.1.7). Thus

$$\theta_4^2(q)=1+4\sum_{n=1}^{\infty}\frac{(-1)^n q^{2n-1}}{1+q^{2n-1}}$$

which is equivalent to (9.1.9).

In the course of his study of Ramanujan's mock theta functions, Andrews [86] discovered the following remarkable cubic counterpart of (9.1.11), which we write as

$$\theta_3^3(q)=8\sum_{n=0}^{\infty}\sum_{j=0}^{2n}\left(\frac{1+q^{4n+2}}{1-q^{4n+2}}\right)q^{(2n+1)^2-(j+1/2)^2}. \tag{9.1.16}$$

It is an easy consequence of (9.1.16) that every number is a sum of three triangular numbers (a fact originally observed by Fermat and proved by Gauss). This also implies that a number is a sum of three odd squares exactly when the number is congruent to 3 modulo 8 (Exercise 7]) as observed by Euler.

Comments and Exercises

A comprehensive account of the development of formulae for sums of $2n$ squares, from elliptic considerations and Lambert series, can be found in Rademacher [73]. Many wonderful related identities are to be found in Ramanujan [62]. Odd sums are much harder to evaluate. They involve generating functions of class numbers as shown in Mordell [16] and Watson [35].

1. Prove Lemma 9.1.

2. Verify (9.1.6) and (9.1.7). Show that these are equivalent to (9.1.8).

3. a) Prove formula (9.1.11) for $\theta_3^2(q)$.
b) Establish (9.1.12) and (9.1.13).

4. a) Let θ tend to π in (9.1.8) and evaluate the limit.
b) Evaluate (9.1.8) when $\theta:=\pi/4,\ \pi/3,\ 2\pi/3$. In particular show that

$$\left[1+6\sum_{n=0}^{\infty}\left(\frac{q^{3n+1}}{1-q^{3n+1}}-\frac{q^{3n+2}}{1-q^{3n+2}}\right)\right]^2=1+12\sum_{3\nmid n}\frac{nq^n}{1-q^n}$$

$$=1+12\sum_{n=1}^{\infty}\frac{q^n}{(1-q^n)^2}-36\sum_{n=1}^{\infty}\frac{q^{3n}}{(1-q^{3n})^2}.$$

5. Two identities due to Lorenz (Dickson [71, vol. 3, p. 29]) are

i) $$\theta_3(q)\theta_3(q^2)=1+2\sum_{\substack{n=1\\ n\text{ odd}}}^{\infty}\chi_8(n)\frac{q^n}{1-q^n}$$

where $\chi_8(n)$ is 1 if $n=8k+1,\ 8k+3$ and -1 if $n=8k+5,\ 8k+7$,

ii) $$\theta_3(q)\theta_3(q^3)=1+2\sum_{n=1}^{\infty}\left(\frac{1-q^n}{1-q^{3n}}\right)q^n+4\sum_{n=1}^{\infty}\left(\frac{1-q^{4n}}{1-q^{12n}}\right)q^{4n}.$$

Let $d_{ai+b}(k)$ be the number of divisors of k of the form $ai+b$.

a) Show that the number $R_2(k)$ of integer solutions of $n^2+2m^2=k$ is given by

$$R_2(k)=2[d_{8i+1}(k)+d_{8i+3}(k)-d_{8i+5}(k)-d_{8i+7}(k)].$$

b) Similarly, the number $R_3(k)$ of integer solutions of $n^2+3m^2=k$ is given by

$$R_3(k)=2[d_{3i+1}(k)-d_{3i+2}(k)]+4[d_{12i+4}(k)-d_{12i+8}(k)].$$

Note that a) follows from Exercise 12 of Section 3.7.

c) Observe that ii) can be used to show that

$$\theta_2(q)\theta_2(q^3)=4\sum_{\substack{n=1\\ n\text{ odd}}}^{\infty}\left(\frac{1-q^{4n}}{1-q^{6n}}\right)q^n=4\sum_{\substack{n=1\\ n\text{ odd}}}^{\infty}\frac{q^n+q^{-n}}{1+q^{2n}+q^{-2n}}.$$

Hence

$$\sum_{n=0}^{\infty}\frac{F_{2n+1}}{1+L_{4n+2}}=\frac{\theta_2(\beta)\theta_2(\beta^3)}{4\sqrt{5}}$$

where $\beta:=(\sqrt{5}-1)/2$ and F_n and L_n are the Fibonacci and Lucas numbers, as in Section 3.7.

6. Use Ramanujan's modular identity of order 3 (Section 5.2) to deduce that

$$1+6\sum_{n=0}^{\infty}\left(\frac{q^{6n+2}}{1-q^{6n+2}}-\frac{q^{6n+4}}{1-q^{6n+4}}\right)=\sqrt{\frac{1}{2}\sum_{i=2}^{4}\theta_i^2(q)\theta_i^2(q^3)}.$$

Hence deduce that

$$\sum_{n=0}^{\infty} \frac{1}{L_{12n+6}-3} = \frac{\sqrt{\frac{1}{2}\sum_{i=2}^{4} \theta_i^2(\beta)\theta_i^2(\beta^3)}-1}{6\sqrt{5}}$$

where $\beta := (3-\sqrt{5})/2$. Note that $\frac{1}{2}\sum_{i=2}^{4}\theta_i^2(q)\theta_i^2(q^3)$ can be written more compactly as $\theta_2^2(q)\theta_2^2(q^3)+\theta_4^2(q^2)\theta_4^2(q^6)$. Find a closed form for the Lambert series above when $q := e^{-\pi/\sqrt{3}}$.

7. Use formula (9.1.16) to establish that every positive integer is the sum of three triangular numbers and that every number of the form $8k+3$ is the sum of three odd squares.

9.2 (CHEMICAL) LATTICE SUMS

Sums of the form

$$b_3(2s) := \sum_{i,j,k=-\infty}^{\infty}{}' \frac{(-1)^{i+j+k}}{(i^2+j^2+k^2)^s} \tag{9.2.1}$$

arise naturally in chemistry. (Here the prime indicates that we avoid summing $i=j=k=0$.) Indeed, $b_3(1)$ can be considered as the potential or Coulomb sum at the origin of a cubic lattice with alternating unit charges at all nonzero lattice points. This may be considered as an idealization of a rocksalt crystal. The quantity $b_3(1)$ is called *Madelung's constant* for NaCl. Different crystals give rise to different lattice sums. We will also consider its two-dimensional (laminar) analogue

$$b_2(2s) := \sum_{i,j=\infty}^{\infty}{}' \frac{(-1)^{i+j}}{(i^2+j^2)^s} \tag{9.2.2}$$

and its four-dimensional form

$$b_4(2s) = \sum_{i,j,k,l=-\infty}^{\infty}{}' \frac{(-1)^{i+j+k+l}}{(i^2+j^2+k^2+l^2)^s}.$$

There are some nontrivial considerations about the sense in which these sums converge. (See Exercises 1 and 2.) We assume all sums denote limits of rectangular summations. These will converge for $\mathrm{re}(s)>0$. The general form of these rectangular sums is

$$\lim_{n\to\infty} s_n := \sum_{i=1}^{N} \sum_{m_i=-n}^{n}{}' (-1)^{\Sigma m_i}\bar{a}(m_1, m_2, \ldots, m_N)$$

which, for real-valued $\bar{a}$, can be shown to converge by an alternating series test. (See Exercise 2.) The convergence in $b_N(1)$ is $O(n^{-1/2})$ so that 10^n terms are needed for $O(n)$ digits. Obviously direct computation is virtually impossible.

Fortunately, some beautiful analytic reductions are possible. In this section we illustrate this for b_2 and b_4. The idea is to observe that, for $\mathrm{re}(s)>0$.

$$\Gamma(s)b_N(2s) = M_s(\theta_4^N - 1) \qquad q := e^{-t} \tag{9.2.3}$$

where M_s is the Mellin transform of Section 3.6. Thus

$$\Gamma(s)b_2(2s) = M_s(\theta_4^2-1) = M_s\left[\left(\sum_{n=-\infty}^{\infty}(-1)^n q^{n^2}\right)^2 - 1\right].$$

Now (9.1.13) shows that

$$\begin{aligned} b_2(2s) &= \Gamma^{-1}(s)4\sum_{n,m=1}^{\infty}(-1)^{n+m-1}M_s[q^{m(2n-1)}] \\ &= 4\sum_{n,m=1}^{\infty}(-1)^{n-1+m}[m(2n-1)]^{-s}. \end{aligned}$$

Thus

$$b_2(2s) = 4\sum_{n=0}^{\infty}\frac{(-1)^n}{(2n+1)^s}\sum_{m=1}^{\infty}\frac{(-1)^m}{m^s} = -4\beta(s)\alpha(s) \tag{9.2.4}$$

and we have factored $b_2(2s)$ into a product of Dirichlet L functions (the alternating ζ function α and $\beta := L_{-4}$) defined by

$$\alpha(s) := \sum_{n=1}^{\infty}\frac{(-1)^{n+1}}{n^s} = (1-2^{1-s})\zeta(s)$$

$$\beta(s) := \sum_{n=0}^{\infty}\frac{(-1)^n}{(2n+1)^s}.$$

In particular, $b_2(2) = -\pi\log 2$. Equation (9.2.4) is originally due to Lorenz. Now any reasonable method of computing $\alpha(\frac{1}{2})$ and $\beta(\frac{1}{2})$ will compute $b_2(1)$. Such is possible by various integral or summation techniques. Correspondingly, from Theorem 3.2,

$$b_4(2s) = \Gamma^{-1}(s)8M_s\left[\sum_{m=1}^{\infty}\frac{m(-q)^m}{1-(-q)^m} - \sum_{m=1}^{\infty}\frac{4mq^{4m}}{1-q^{4m}}\right]$$

and expansion gives

$$b_4(2s) = \Gamma^{-1}(s)\left[8 \sum_{m,k=1}^{\infty} (-1)^{mk} m M_s(q^{mk}) - 8 \sum_{m,k=1}^{\infty} 4mM_s(q^{4mk})\right].$$

Now we compute these transforms and have

$$b_4(2s) = 8 \sum_{m,k=1}^{\infty} \frac{[(-1)^{mk} - 1]m}{(mk)^s} + 8(1 - 4^{1-s}) \sum_{m,k=1}^{\infty} \frac{m}{(mk)^s}$$

on adding and subtracting $m(mk)^{-s}$ in each summation. Thus

$$b_4(2s) = -16 \sum_{n=0}^{\infty} \frac{1}{(2n+1)^s} \sum_{m=0}^{\infty} \frac{1}{(2m+1)^{s-1}} + 8(1 - 4^{1-s})\zeta(s-1)\zeta(s).$$

But $\Sigma_{n=0}^{\infty} (2n+1)^{-s} = (1 - 2^{-s})\zeta(s)$ and so

(9.2.5) $b_4(2s) = -8(1 - 2^{2-s})(1 - 2^{1-s})\zeta(s)\zeta(s-1) = -8\alpha(s)\alpha(s-1)$.

In particular,

$$b_4(2) = -4\log 2 = \frac{4}{\pi}\, b_2(2).$$

Use of the functional equation for ζ, equation (3.6.6), allows one to establish other formulae. In general any identity for any even-dimensional power of theta functions will convert into a factorization for a matching lattice sum. (See Exercise 4.) In Exercises 6 through 10 we show how two-dimensional lattice sums may be used to evaluate elliptic invariants.

Comments and Exercises

An excellent and extensive recent survey of lattice sums can be found in Glasser and Zucker [80]. This also discusses their chemical origin at some length. Madelung's constant is analyzed from a mathematical perspective in Borwein, Borwein, and Taylor [85]. There is ambiguity in the literature as to whether the constants are positive or negative. We have chosen the sign as convenient.

1. (*Analyticity of lattice sums*)

a) Considered as a limit of rectangular sums, show that $b_2(s)$ and $b_3(s)$ exist and are analytic for $\mathrm{re}(s) > 0$.
Hint: Use the Mellin transform.

b) Show that

$$b_2(2s) = \sum_{n=1}^{\infty} (-1)^n \frac{r_2(n)}{n^s} \qquad \mathrm{re}(s) > \frac{1}{3}.$$

Hint: $g_2(2s) := \Sigma_{n=1}^{\infty} (-1)^n r_2(n) n^{-s}$ converges and is analytic for $\mathrm{re}(s) > \frac{1}{3}$. For $\mathrm{re}(s) > 1$, $g_2(2s)$ and $b_2(2s)$ coincide.

c) The analogous sum $g_3(2s) := \Sigma_{n=1}^{\infty} (-1)^n r_3(n) n^{-s}$ diverges for $s := \frac{1}{2}$.

2. (*Alternating series test*) A mapping $\bar{a}: \mathbb{N}^N \to \mathbb{R}$ is (N-)*monotone* if, for $m_1, m_2, \ldots, m_N \geq 0$,

$$\sum_{i=1}^{N} \sum_{s_i=0,1} (-1)^{\Sigma s_i} \bar{a}(m_1 + s_1, m_2 + s_2, \ldots, m_N + s_N) \geq 0.$$

Thus 1-monotonicity is just $\bar{a}(m) \geq \bar{a}(m+1)$, and 2-monotonicity is $\bar{a}(m,n) + \bar{a}(m+1, n+1) \geq \bar{a}(m, n+1) + \bar{a}(m+1, n)$, while 3-monotonicity demands that the alternating sum over any unit cube be positive if the bottom corner is. We say that $\bar{a}$ is *fully monotone* if $\bar{a}$ and all its restrictions are monotone. Consider

$$\sum_{i=1}^{N} \sum_{m_i=0}^{\infty} (-1)^{\Sigma m_i} \bar{a}(m_1, m_2, \ldots, m_N).$$

a) Prove the following alternating series test given in D. Borwein and J. Borwein [86]. If $\bar{a}$ is fully monotone and $\lim_{\bar{m}\to\infty} \bar{a}(\bar{m}) = 0$, then the rectangular sums converge alternatingly. *Hint*: (In two dimensions) show that $s_n := \Pi_{i,j=0}^{n} (-1)^{i+j} \bar{a}(i,j)$ satisfies

i) $s_{2n} \geq s_{2n+2}$
ii) $s_{2n+1} \geq s_{2n-1}$
iii) $S_{2n} - S_{2n-1} \to 0$

Draw a picture. (The case of b_3 and b_2 is spelt out in Borwein, Borwein, and Taylor [85]. An analogous bounded convergence test due to Hardy can be found in Bromwich [26].)

b) Suppose that $\bar{a}$ is N times continuously differentiable on $(\mathbb{R}^+)^N$. Show that $\bar{a}$ is totally monotone if the partial derivatives satisfy

$$\bar{a}_{i_1} \leq 0,\ \bar{a}_{i_1 i_2} \geq 0,\ \bar{a}_{i_1 i_2 i_3} \leq 0, \ldots, (-1)^N \bar{a}_{i_1 i_2 \ldots i_N} \geq 0$$

for all partial derivatives with $i_1 < i_2 < i_3 < \cdots < i_N$.

c) Verify that $\Sigma_0^{\infty} (-1)^{i+j+k}(i^2 + j^2 + k^2)^{-p}$ and $\Sigma_0^{\infty} (-1)^{i+j}(2i+j)^{-p}$ converge for $p > 0$.

3. Prove that $\Gamma(s) b_N(s) = M_s(\theta_4^N - 1)$.

4. a) Show that

$$\sum_{-\infty}^{\infty}{}' \frac{1}{(n^2 + m^2)^s} = 4\beta(s)\zeta(s) \qquad \mathrm{re}(s) > 1$$

and

$$\sum_{-\infty}^{\infty}{}' \frac{(-1)^n}{(n^2 + m^2)^s} = 2^{-s} b_2(2s) \qquad \mathrm{re}(s) > 1.$$

b) Show that

$$b_8(2s) = -16\zeta(s)\alpha(s-3) \qquad \mathrm{re}\,(s) > 1$$

is equivalent to the formula (3.2.25)

$$\theta_4^8(q) = 1 + 16\sum_{n=1}^{\infty} \frac{(-1)^n n^3 q^n}{1-q^n}. \tag{9.2.6}$$

c) Use $\theta_2\theta_3\theta_4 = \theta_1^+$, equation (3.2.4), to show that

$$\sum_{-\infty}^{\infty} \frac{(-1)^m}{[m^2+n^2+(p+\frac{1}{2})^2]^s} = 2^{2s+1}\beta(2s-1). \tag{9.2.7}$$

5. The hexagonal sum is

$$h_2(2s) := \sum_{-\infty}^{\infty}{}' \frac{q(n,m)}{[(n+m/2)^2+3(m/2)^2]^s} \qquad \mathrm{re}(s) > 0$$

where $q(n,m) := \frac{4}{3}\{\sin[(n+1)\theta]\sin[(m+1)\theta] - \sin(n\theta)\sin[(m-1)\theta]\}$ and $\theta := 2\pi/3$. This corresponds to calculating the Coulomb potential on a regular hexagonal lattice. (See Borwein, Borwein, and Taylor [85].)

a) For $\mathrm{re}(s) > 1$, show using the cubic modular equation that

$$h_2(2s) = \left(\frac{1-3^{1-s}}{2}\right)\left[2\sum{}' \frac{1}{(n^2+3m^2)^s} - \sum{}' \frac{(-1)^{n+m}}{(n^2+3m^2)^s}\right].$$

b) A formula of Cauchy (Dickson [71, vol. 3, p. 20]) gives

$$\theta_4(q)\theta_4(q^3) = 1 + 2\sum_{n=1}^{\infty}(-1)^n q^n\left[\frac{1+q^n}{1+q^{3n}}\right].$$

Use this and a) to deduce that

$$h_2(2s) = 3(1-3^{1-s})\zeta(s)L_{-3}(s)$$

where

$$L_{-3}(s) := 1 - 2^{-s} + 4^{-s} - 5^{-s} + 7^{-s} - 8^{-s} + \cdots.$$

c) This provides an analytic continuation of $h_2(2s)$. Thus

$$3(\sqrt{3}-1)(\sqrt{2}+1)\alpha(\tfrac{1}{2})L_{-3}(\tfrac{1}{2}) = h_2(1)$$

is Madelung's constant for the hexagonal lattice. Show that

$$h_2(2) = \sqrt{3}\pi \log 3.$$

6. (*Evaluating invariants*) The factorization of two-dimensional zeta sums into sums of products of L series can be carried a great deal further. This is described in Glasser and Zucker [80] and in Zucker and Robertson [76*a*,*b*]. By combining number theoretic and transform techniques, one can explicitly factor all sums whose discriminants are *disjoint* (have one form per genus) and a few others. This leads to formulae such as

$$\sum{}'(m^2+Pn^2)^{-s} = 2^{1-t}\sum_{\mu|P} L_{\pm\mu}L_{\mp4P/\mu} \tag{9.2.8}$$

and

$$\sum{}'(m^2+2Pn^2)^{-s} = 2^{1-t}\sum_{\mu|P} L_{\pm\mu}L_{\mp8P/\mu}. \tag{9.2.9}$$

In these two formulae P is an odd square-free number [congruent to 1 modulo 4 in (9.2.8)] with t distinct factors. The right hand sums over all divisors of P and one has

$$L_{\pm d}(s) := \sum_{n=1}^{\infty}(\pm d|n)n^{-s}$$

which are primitive L series modulo d. (These can only exist for $d = P$, $4P$, or $8P$, and the sign configuration is in fact uniquely specified.) Here $(k|n)$ is the *Kronecker* (*generalized Legendre*) symbol. $L_{\pm\mu}$ is taken for $\mu \equiv \pm1 \pmod 4$. For example, with $P := 29$, (9.2.8) becomes

$$\sum{}'(m^2+29n^2)^{-s} = L_1L_{-116} + L_{-4}L_{29}.$$

Dickson [29] gives an extensive list of disjoint discriminants. In particular, there are 18 numbers less than 10,000 to which (9.2.8) applies and 15 numbers less than 10,000 to which (9.2.9) applies. Indeed, (9.2.8) holds for *type one* $P :=$ 5, 13, 21, 33, 37, 57, 85, 93, 105, 133, 165, 177, 253, 273, 345, 357, 385, 1365 and (9.2.9) holds for *type two* $P :=$ 1, 3, 5, 11, 15, 21, 29, 35, 39, 51, 65, 95, 105, 165, 231. There are only finitely many disjoint discriminants. We shall call such *P solvable*.

Implicit in (9.2.8) and (9.2.9) are corresponding theta series identities, and formulae for representations as weighted sums of squares.

a) Show that if q is replaced by $-q$ in (9.2.8) and (9.2.9), we produce formulae for

i) $\sum{}'(-1)^{m+n}(m^2+Pn^2)^s$

ii) $\sum{}'(-1)^m(m^2+2Pn^2)^{-s}$.

b) Show that the effect of replacing q by $-q$ in (9.2.8), (9.2.9), or similar formulae is to replace $L_{\pm d}$ by $-[1-(2|d)2^{1-s}]L_{\pm d}$, unless the L function was multiplied by some factor involving 2^{-s}, or d is even, in which cases it is unchanged.

c) Recall that (3.2.12) and Exercise 4d) of Section 3.2 gave

$$\sum{}' (-1)^{m+n}(m^2+rn^2)^{-1} = -\frac{4\pi}{\sqrt{r}} \log f(\sqrt{-r})$$

and

$$\sum{}' (-1)^{m}(m^2+rn^2)^{-1} = -\frac{4\pi}{\sqrt{r}} \log f_1(\sqrt{-r})\,.$$

Use these formulae with a) and b) to establish that for the appropriate P,

i) $$2^{t-1}\frac{\pi}{\sqrt{P}} \log f^4(\sqrt{-P}) = L_{-4P}(1)\log 2 + \sum_{\substack{\mu|P\\ \mu\neq 1}} [1-(2|\mu)]L_{\pm\mu}(1)L_{\mp 4P/\mu}(1)$$

ii) $$2^{t-1}\frac{\pi}{\sqrt{2P}} \log f_1^4(\sqrt{-2P}) = L_{-8P}(1)\log 2 + \sum_{\substack{\mu|P\\ \mu\neq 1}} [1-(2|\mu)]L_{\pm\mu}(1)L_{\mp 8P/\mu}(1).$$

d) The classical Dirichlet class number formulae (Landau [58]) allow us to write $L_{\pm d}(1)$ algebraically. One has, for $d>0$ restricted so that $L_{\pm d}$ is primitive,

i) $$L_{+d}(1) = 2\frac{h(d)}{\sqrt{d}}\log \varepsilon(d)$$

ii) $$L_{-d}(1) = \frac{2\pi}{\sqrt{d}}\frac{h(-d)}{w(d)}\,.$$

Here $h(d)$ is the number of (broadly) equivalent primitive classes of reduced forms with discriminant $d=b^2-4ac$ or ideals in $\mathbb{Q}(\sqrt{D})$ where d is D or $4D$, depending on whether $D\equiv 1 \pmod 4$ or $D\equiv 2,3 \pmod 4$; $\varepsilon(d)$ is the *fundamental unit* in $\mathbb{Q}(\sqrt{D})$, which may be computed from the fundamental solution of the appropriate Pell's equation (see LeVeque [77] and Hua [82]); and $w(d)$ is a factor which counts the number of automorphs of the form, and is 2 except that $w(3)=6$ and $w(4)=4$. From formula (4.12) in Zucker and Robertson [76*a*] we have Dirichlet's formulae, for $d>4$,

$$h(-d) = \frac{-1}{d}\sum_{n=1}^{d-1} n(-d|n)\,.$$

Also for $d>0$

$$h(d)\log\varepsilon(d) = -\frac{1}{2}\sum_{n=1}^{d-1}(d|n)\log\left(\sin\left(\frac{n\pi}{d}\right)\right).$$

Moreover, for disjoint forms, one can observe that the class number $h(-d)$ must coincide with the number of *genera* g. The number of genera is as follows. If d is odd, then $g=2^{m-1}$, where d has m distinct prime factors. If d is even and $d/4$ has m distinct prime factors (including 2), then $g=2^m$ when $d/4\equiv 0,1,5 \pmod 8$ and $g=2^{m-1}$ otherwise.

An excellent brief survey of history and of recent advances regarding the class number can be found in Goldfeld [85]. Now observe that, for the appropriate P, both $\frac{1}{2}f^4$ and $\frac{1}{2}f_1^4$ will be products of powers of fundamental units from some of the divisors of $4P$ or $8P$. [For our solvable P, $h(-4P)=2^t$ when $P\equiv 1 \pmod 4$ and $h(-8P)=2^t$.] In particular, verify that for $P:=5$, 13, or 37, since $t=1$ in each case

$$G_P^4 = \tfrac{1}{2}f_1^4(\sqrt{-P}) = \varepsilon(P)^{h(P)}\,.$$

Since $h(P)=1$ in each case, we see that

$$G_5^4 = \frac{\sqrt{5}+1}{2} \qquad G_{13}^4 = \frac{\sqrt{13}+3}{2} \qquad G_{37}^4 = \sqrt{37}+6\,.$$

Similarly, we may now verify the values of G_P^6, $P:=21, 33, 57, 93$, given in Exercise 9 and 10 of Section 4.7.

e) Establish that for $P:=5$ or 29,

$$g_{2P}^2 = \varepsilon(P)\,,$$

and for $P:=3$ or 11,

$$g_{2P}^{w(P)} = \varepsilon(2)\,.$$

(Compare Table 5.2.)

For all the type one numbers P listed above, we can now explicitly give G_p. Similarly for the type two numbers we can give g_{2P}. This accounts for most of the square-free and nonprime invariants given by Weber or Ramanujan.

f) Show that

$$g_{130}^2 = \left(\frac{\sqrt{5}+1}{2}\right)^3\left(\frac{\sqrt{13}+3}{2}\right).$$

7. (*Evaluating singular values*) We can proceed further to evaluate $k := \lambda^*(2P)$ for P of type two. We know that $k/4 = f_1^4(\sqrt{-2P})f_1^{-8}(\sqrt{-8P})$. Hence

$$-\frac{\pi}{\sqrt{2P}}\log\left(\frac{k}{4}\right) = \sum{}'(-1)^m(m^2+2Pn^2)^{-1} - 4\sum{}'(-1)^m(m^2+8Pn^2)^{-1}.$$

We already know [Exercise 6c)] the first sum on the right. From some elementary, but skillful, theta transformations we may deduce that

$$2^t\sum{}'(-1)^m(m^2+8Pn^2)^{-s} = \sum_{\mu|P}\{[2^{1-2s}-1+2^{-s}(2|\mu)]L_{\pm\mu}L_{\mp 8P/\mu} + L_{\mp 4\mu}L_{\pm 8P/\mu}\}.$$

On setting $s := 1$ and substituting above, we derive

(9.2.10) $$-\frac{\pi}{\sqrt{2P}}\log k = 2^{2-t}\sum_{\mu|P}L_{\pm 4\mu}(1)L_{\mp 8P/\mu}(1),$$

a beautiful simplification.

a) Use (9.2.10) to compute $\lambda^*(2P)$ for $P := 3, 5, 11, 29$.
b) Use (9.2.10) to compute $\lambda^*(210)$ given in (4.6.12).
c) Observe, as Zucker did, that there are computable in this form two larger singular values: those for $2P := 330$ and 462. Verify that

(9.2.11) $$\lambda^*(330) = (2-\sqrt{3})^3(\sqrt{2}-1)^2(\sqrt{33}-4\sqrt{2})^2(\sqrt{10}-3)^2 \times(3\sqrt{5}-2\sqrt{11})^2(4-\sqrt{15})(\sqrt{55}-3\sqrt{6})(10-3\sqrt{11})$$

and that

(9.2.12) $$\lambda^*(462) = (\sqrt{3}-\sqrt{2})^4(2-\sqrt{3})^2(2\sqrt{2}-\sqrt{7})^2(8-3\sqrt{7})^2 \times(3\sqrt{11}-7\sqrt{2})^2(\sqrt{22}-\sqrt{21})(10-3\sqrt{11})(76-5\sqrt{231}).$$

8. (*Evaluation of* K *in terms of* Γ) Selberg and Chowla [67] showed for all rational numbers r that $K(\lambda^*(r))$ is expressible in closed form using a finite number of Γ values. This relied on Kronecker's remarkable 'Grenz-Formel,' which has

(9.2.13) $$\lim_{s\downarrow 1}\left\{\sum{}'(m^2+rn^2)^{-s} - \frac{\pi}{(s-1)\sqrt{r}}\right\} = \frac{\pi}{\sqrt{r}}[2\gamma - \log(4r) - 4\log\eta]$$

as a special case. Here $\eta := \eta(\sqrt{-r})$ is the eta function of (3.2.9) and (3.2.11), and γ is Euler's constant. Using (9.2.13), Zucker [77] applies the factorization results described above to explicitly compute K corresponding to solvable sums in terms of π, surds, and Γ values. This leads to the following table of evaluations (Table 9.1). Elsewhere Zucker has actually given $K(\lambda^*(210))$ [which involves $\Gamma(n/840)$ for $(n, 840) = 1$]. The general formula valid for either $r := P$ (P of type one) or $r := 2P$ (P of type two) is given by

$$K = \frac{\pi}{2}\eta^2 f^4$$

and

(9.2.14) $$4\log\eta(\sqrt{-r}) = \frac{1}{h(-4r)}\sum_{n=1}^{4r-1}(-4r|n)\Gamma\left(\frac{n}{4r}\right) - \log(8\pi r) - \frac{2\sqrt{r}}{\pi h(-4r)}\sum_{\substack{\mu|P\\ \mu\neq 1}}L_{\pm\mu}(1)L_{\mp 4r/\mu}(1).$$

There is a corresponding formula when in Zucker's terms $S(1, 1, (1+r)/4)$ is solvable.

a) Verify the contents of Table 9.1, for $r = 1, 2, \ldots, 6$.
b) Show that $\Gamma(m/24)$ is $0_{\text{op}}(\log n)$ computable for integral m. *Hint*: Express such Γ values in terms of K at singular values. It would be interesting to know if this is possible more generally.
c) Compute $E((3-\sqrt{7})/4\sqrt{2})$. (Compare Exercise 9 of Section 5.2.)
d) Show in general that $E(\lambda^*(r))$ is computable in terms of Γ values and algebraic quantities for rational r.

9. (*Conjugate divisors and evaluations of* k) Consider P as above and suppose $P := d_1d_2$ and $Q := d_1/d_2$ for divisors d_1 and d_2. Using Kronecker's genus character sum formulae one can show that G_P and $G_Q = G_{Q^{-1}}$ must have the same general form for P of type one. Similarly, g_{2P} and $g_{2Q} = g^{-1}_{2Q^{-1}}$ are paired, as are $\lambda^*(2P)$ and $\lambda^*(2Q)$. This is best illustrated with examples.

a) Show that

$$g_{190}^2 = (\sqrt{5}+2)(\sqrt{10}+3) \qquad g_{38/5}^2 = (\sqrt{5}-2)(\sqrt{10}+3).$$

The first value may be computed as above. The second is easily verified from Schlafli's form of the quintic modular equation.

TABLE 9.1. Evaluation of K at the First Sixteen Singular Values

r	K
1	$\dfrac{[\Gamma(\frac14)]^2}{4\pi^{1/2}}$
2	$\dfrac{(\sqrt2+1)^{1/2}\Gamma(\frac18)\Gamma(\frac38)}{2^{13/4}\pi^{1/2}}$
3	$\dfrac{3^{1/4}[\Gamma(\frac13)]^3}{2^{7/3}\pi}$
4	$\dfrac{(\sqrt2+1)[\Gamma(\frac14)]^2}{2^{7/2}\pi^{1/2}}$
5	$(\sqrt5+2)^{1/4}\left[\dfrac{\Gamma(\frac{1}{20})\Gamma(\frac{3}{20})\Gamma(\frac{7}{20})\Gamma(\frac{9}{20})}{160\pi}\right]^{1/2}$
6	$\left[\dfrac{(\sqrt2-1)(\sqrt3+\sqrt2)(2+\sqrt3)\Gamma(\frac{1}{24})\Gamma(\frac{5}{24})\Gamma(\frac{7}{24})\Gamma(\frac{11}{24})}{384\pi}\right]^{1/2}$
7	$\dfrac{\Gamma(\frac17)\Gamma(\frac27)\Gamma(\frac47)}{(7^{1/4})4\pi}$
8	$\left[\dfrac{2\sqrt2+(1+5\sqrt2)^{1/2}}{4\sqrt2}\right]^{1/2}\dfrac{(\sqrt2+1)^{1/2}\Gamma(\frac18)\Gamma(\frac38)}{8\pi^{1/2}}$
9	$\dfrac{3^{1/4}(2+\sqrt3)^{1/2}}{12\pi^{1/2}}\left[\Gamma\left(\dfrac14\right)\right]^2$
10	$\left[\dfrac{(2+3\sqrt2+\sqrt5)\Gamma(\frac{1}{40})\Gamma(\frac{7}{40})\Gamma(\frac{9}{40})\Gamma(\frac{11}{40})\Gamma(\frac{13}{40})\Gamma(\frac{19}{40})\Gamma(\frac{23}{40})\Gamma(\frac{37}{40})}{2560\pi^3}\right]^{1/2}$
11	$[2+(17+3\sqrt{33})^{1/3}+(17-3\sqrt{33})^{1/3}]^2\,\dfrac{\Gamma(\frac{1}{11})\Gamma(\frac{3}{11})\Gamma(\frac{4}{11})\Gamma(\frac{5}{11})\Gamma(\frac{9}{11})}{(11^{1/4})144\pi^2}$
12	$\dfrac{(\sqrt2+1)(\sqrt3+\sqrt2)(2-\sqrt3)^{1/2}3^{1/4}[\Gamma(\frac13)]^3}{2^{13/3}\pi}$
13	$(18+5\sqrt{13})^{1/4}\times\left[\dfrac{\Gamma(\frac{1}{52})\Gamma(\frac{7}{52})\Gamma(\frac{9}{52})\Gamma(\frac{11}{52})\Gamma(\frac{15}{52})\Gamma(\frac{17}{52})\Gamma(\frac{19}{52})\Gamma(\frac{25}{52})\Gamma(\frac{29}{52})\Gamma(\frac{31}{52})\Gamma(\frac{47}{52})\Gamma(\frac{49}{52})}{6656\pi^5}\right]^{1/2}$
14	$[(10+6\sqrt2)^{1/2}+(2+2\sqrt2)^{1/2}+(3+\sqrt2)^{1/2}]^{1/2}\times\dfrac{[\Gamma(\frac{1}{56})\Gamma(\frac{3}{56})\Gamma(\frac{9}{56})\Gamma(\frac{13}{56})\Gamma(\frac{15}{56})\Gamma(\frac{19}{56})\Gamma(\frac{23}{56})\Gamma(\frac{25}{56})\Gamma(\frac{27}{56})\Gamma(\frac{39}{56})\Gamma(\frac{45}{56})]^{1/2}}{16\pi\sqrt7}$
15	$\left[\dfrac{(\sqrt5+1)\Gamma(\frac{1}{15})\Gamma(\frac{2}{15})\Gamma(\frac{4}{15})\Gamma(\frac{8}{15})}{240\pi}\right]^{1/2}$
16	$\dfrac{(2^{1/4}+1)^2[\Gamma(\frac14)]^2}{2^{9/2}\pi^{1/2}}$

b) Correspondingly

$$G_{105}^6=\left(\frac{\sqrt5+1}{2}\right)^3\left(\frac{\sqrt3+1}{\sqrt2}\right)^3\left(\frac{\sqrt7+\sqrt3}{2}\right)^3\left(\frac{\sqrt7+\sqrt5}{\sqrt2}\right)$$

$$G_{35/3}^6=\left(\frac{\sqrt5-1}{2}\right)^3\left(\frac{\sqrt3+1}{\sqrt2}\right)^3\left(\frac{\sqrt7+\sqrt3}{2}\right)^3\left(\frac{\sqrt7-\sqrt5}{\sqrt2}\right)$$

$$G_{21/5}^6=\left(\frac{\sqrt5+1}{2}\right)^3\left(\frac{\sqrt3-1}{\sqrt2}\right)^3\left(\frac{\sqrt7+\sqrt3}{2}\right)^3\left(\frac{\sqrt7-\sqrt5}{\sqrt2}\right)$$

$$G_{15/7}^6=\left(\frac{\sqrt5-1}{2}\right)^3\left(\frac{\sqrt3-1}{\sqrt2}\right)^3\left(\frac{\sqrt7+\sqrt3}{2}\right)^3\left(\frac{\sqrt7+\sqrt5}{\sqrt2}\right).$$

One may verify $G_{35/3}$ and $G_{21/5}$ from the corresponding cubic and quintic equations, and so on.

c) Use the techniques of Section 5.3 to compute $\sigma(105)$.

d) Observe that

i) $\lambda^*(6)=(2-\sqrt3)(\sqrt3-\sqrt2)$
$\lambda^*(\frac23)=\lambda^{*\prime}(\frac32)=(2-\sqrt3)(\sqrt3+\sqrt2)$

ii) $\lambda^*(10)=(\sqrt{10}-3)(\sqrt2-1)^2$
$\lambda^*(\frac25)=\lambda^{*\prime}(\frac52)=(\sqrt{10}-3)(\sqrt2+1)^2$

iii) $\lambda^*(58)=(13\sqrt{58}-99)(\sqrt2-1)^6$
$\lambda^*(\frac{2}{29})=\lambda^{*\prime}(\frac{29}{2})=(13\sqrt{58}-99)(\sqrt2+1)^6$.

e) Indeed, for all P of type two, $\lambda^*(2Q)$ and $\lambda^*(2P)$ will be "conjugate", as we illustrate for $\lambda^*(210)$. Let

$$u_1:=(\sqrt2-1)^2\qquad u_2:=(\sqrt7-\sqrt6)^2\qquad u_3:=(\sqrt{10}-3)^2$$
$$u_4:=(4-\sqrt{15})^2\qquad u_5:=2-\sqrt3\qquad u_6:=\sqrt{15}-\sqrt{14}$$
$$u_7:=6-\sqrt{35}\qquad u_8:=8-3\sqrt7\,.$$

Then $\lambda^*(210)=\prod_{m=1}^8 u_m$, and each $\lambda^*(2Q)$ is a corresponding product $\prod_{m=1}^8 u_m^{\varepsilon_m(Q)}$ where each ε_m is ±1. In compact form one has $\varepsilon_m(Q):=1-2b^m(Q)$, where $b^m(Q)$ is the mth binary digit of $b(2Q)$ defined by

$$b(\tfrac{70}{3})=142\qquad b(\tfrac{42}{5})=201\qquad b(\tfrac{30}{7})=45$$
$$b(\tfrac{14}{15})=71\qquad b(\tfrac{10}{21})=163\qquad b(\tfrac{6}{35})=228$$
$$b(\tfrac{2}{105})=106\qquad b(210)=0\,.$$

These correspond to all the reduced forms with discriminant 840.

f) Numerically, find the "conjugate" values for $P:=165$ and $P:=231$. [This involves computing 2^8 products and comparing them with the theta expansion of $k(2Q)$.]

With these conjugate values and the formulae of Section 5.3 one may observe that $\alpha(2P)$ is now available in closed form for all P of type two (and for conjugate divisors Q). Again we illustrate with an exercise.

10. a) Generate a recursive version of formula (5.3.3) and specialize this expression to produce a formula for $\alpha(2d_1d_2)$ in terms of R_{d_1}, R_{d_2}, M_{d_2}, M_2 and the appropriate singular values.

b) Apply this formula with $d_1:=35$ and $d_2:=3$ to compute $\alpha(210)$. Observe that this uses only values of λ^* given in Exercise 9e).

c) Compute $\alpha(42)$. *Note*: $g_{42}^6=(2\sqrt{2}+\sqrt{7})[(\sqrt{7}+\sqrt{3})/2]^3$ is incorrectly given in Weber [08].

11. Let $\{a_n\}$ and $\{b_n\}$ be given sequences.

a) Show that

$$\zeta(s)\sum_{n=1}^{\infty} a_n n^{-s}=\sum_{n=1}^{\infty} b_n n^{-s}$$

if and only if

$$\sum_{n=1}^{\infty} a_n \frac{x^n}{1-x^n}=\sum_{n=1}^{\infty} b_n x^n .$$

b) Show that

$$\alpha(s)\sum_{n=1}^{\infty} a_n n^{-s}=\sum_{n=1}^{\infty} b_n n^{-s}$$

if and only if

$$\sum_{n=1}^{\infty} a_n \frac{x^n}{1+x^n}=\sum_{n=1}^{\infty} b_n x^n .$$

c) Show that, with the notation of Exercise 12 of Section 3.7,

i) $\displaystyle\sum_{n=1}^{\infty}\sigma_k(n)n^{-s}=\zeta(s-k)\zeta(s)$

and

ii) $\displaystyle\sum_{n=1}^{\infty}e(n)n^{-s}=\frac{\zeta(2s)}{\zeta(s)}$.

Also

iii) $\displaystyle\sum_{n=1}^{\infty}\phi(n)n^{-s}=\frac{\zeta(s-1)}{\zeta(s)}$

where ϕ is Euler's *totient* function, which counts the numbers less than n and relatively prime to n. Thus $\phi(1):=1$, $\phi(5)=4$, and $\phi(6)=2$.

9.3 *ODD-DIMENSIONAL SUMS AND BENSON'S FORMULA*

While even-dimensional sums usually factor, only a few odd-dimensional ones factor. The reader can, however, produce identities like (9.2.7) from Jacobi's identity (3.1.15) or from (3.2.8). (See Exercise 1.) There are nonetheless many theta-based techniques of which we establish one based on the theta transform.

Theorem 9.1 **(*Benson* (*1956*))**

$$-b_3(1)=\sum_{-\infty}^{\infty}{}' \frac{(-1)^{i+j+k+1}}{(i^2+j^2+k^2)^{1/2}}=12\pi\sum_{\substack{m,n=1\\ \text{odd}}}^{\infty}\operatorname{sech}^2\left[\frac{\pi}{2}(m^2+n^2)^{1/2}\right]. \tag{9.3.1}$$

Proof. By symmetry,

$$b_3(1)=3\sum_{-\infty}^{\infty}{}' \frac{(-1)^i i^2(-1)^{j+k}}{(i^2+j^2+k^2)^{3/2}}$$

and

$$\Gamma\left(\frac{3}{2}\right)b_3(1)=3\sum_{n=-\infty}^{\infty}(-1)^n n^2 M_{3/2}\left[\sum_{j,k=-\infty}^{\infty}(-1)^{j+k}q^{n^2+j^2+k^2}\right]$$

where $q:=e^{-t}$. Thus

$$\Gamma\left(\frac{3}{2}\right)b_3(1)=3M_{3/2}\left[\sum_{-\infty}^{\infty}(-1)^n n^2 q^{n^2}\theta_4^2(t)\right].$$

The theta transform (2.3.2) leads to

$$-\Gamma\left(\frac{3}{2}\right)b_3(1)=3M_{3/2}\left[\sum_{-\infty}^{\infty}(-1)^{n+1}n^2 q^{n^2}\frac{\pi}{t}\theta_2^2\left(\frac{\pi^2}{t}\right)\right]$$

and since $\Gamma(\frac{3}{2}) = \sqrt{\pi}/2$,

$$-b_3(1) = 12\sqrt{\pi} \sum_{n=1}^{\infty} \left\{(-1)^{n+1} n^2 \sum_{\substack{j,k=-\infty \\ \text{odd}}}^{\infty} \int_0^{\infty} [e^{-n^2 t - (\pi^2/4t)(j^2+k^2)}] t^{-1/2}\, dt\right\}.$$

The internal integral $I(n, j, k)$ was evaluated in Exercise 4 of Section 2.2. We have

$$\left(\frac{\pi}{n^2}\right)^{1/2} e^{-\pi n\sqrt{j^2+k^2}} = I(n, j, k)$$

and

$$-b_3(1) = 48\pi \sum_{j,k=0}^{\infty} \sum_{n=1}^{\infty} (-1)^{n+1} n e^{-\pi n\sqrt{(2j+1)^2+(2k+1)^2}}.$$

Finally, for $a > 0$,

$$4\sum_{n=1}^{\infty} (-1)^{n+1} n e^{-an} = \frac{4e^{-a}}{(1+e^{-a})^2} = \operatorname{sech}^2\left(\frac{a}{2}\right)$$

and Benson's formula follows. □

The convergence acceleration is astounding. Summing for $0 \le j,\ k \le 3$ produces $b_3(1) := -1.74756459\ldots$, which is correct to eight places. Even the first approximation, by $-12\pi \operatorname{sech}^2(\pi/\sqrt{2})$, gives $-1.73\ldots$.

For $s \neq \frac{1}{2}$ this manipulation leads to an integral involving Bessel functions of the second kind, and the closed form is lost. There is, however, an extension to N dimensions (among others). One can show that

$$\text{(9.3.2)} \qquad -b_N(N-2) = \frac{2^{N-2}N}{\Gamma(N/2)} \pi^{N/2} \sum_{i=2}^{N} \sum_{\substack{k_i=1 \\ \text{odd}}}^{\infty} \operatorname{sech}^2\left(\frac{\pi}{2}\sqrt{\sum_{i=2}^{N} k_i^2}\right).$$

Thus

$$\text{(9.3.3)} \qquad -b_4(1) = 16\pi^2 \sum_{\substack{i,j,k=1 \\ \text{odd}}}^{\infty} \operatorname{sech}^2\left(\frac{\pi}{2}\sqrt{i^2+j^2+k^2}\right) = 4\log 2$$

and

$$\text{(9.3.4)} \qquad -b_2(0) = 2\pi \sum_{n=0}^{\infty} \operatorname{sech}^2\left[\frac{\pi}{2}(2n+1)\right] = 1$$

which coincides with Exercise 7eii) of Section 3.7. (See Exercise 2.) For the final evaluation it helps to know that for primitive L series

$$L_{-k}(0) = \frac{\sqrt{k}}{\pi} L_{-k}(1)$$

as follows from the functional equations for $L_{\pm k}$:

$$L_{-k}(s) = C(s)\cos\left(\frac{s\pi}{2}\right) L_{-k}(1-s)$$

$$L_{+k}(s) = C(s)\sin\left(\frac{s\pi}{2}\right) L_{+k}(1-s)$$

where $C(s) := 2^s \pi^{s-1} k^{-s+1/2}\Gamma(1-s)$.

Comments and Exercises

Our derivation of Benson's formula can be found in Glasser and Zucker [80]. In that paper, and references therein, one finds much further discussion of odd-dimensional sums. They also illuminate the relationship between the multidimensional zeta functions of Epstein and lattice sums.

1. a) Show that

$$2\sum_{-\infty}^{\infty} (-1)^m \left[\left(2m - \frac{1}{2}\right)^2 + 2n^2 + 2p^2\right]^{-s} = 2^{s+1} L_{-8}(2s-1)$$

where $L_{-8}(s) := 1 + 3^{-s} - 5^{-s} - 7^{-s} + \cdots$.

b) Show that

$$g(2s) := \sum_{-\infty}^{\infty} (-1)^{m+n+p} \left[\left(m+\frac{1}{6}\right)^2 + \left(n+\frac{1}{6}\right)^2 + \left(p+\frac{1}{6}\right)^2\right]^{-s}$$

$$= 12^s \beta(2s-1)$$

and $g(1) = \sqrt{12}\beta(0) = \sqrt{3}$.

c) Derive similar identities from Exercise 5 of Section 4.7.

2. Establish the generalization of Benson's formula (9.3.2) and its special cases (9.3.3) and (9.3.4). Exercise 4b) of Section 9.2 shows that $b_8(6) = -8\zeta(3)$.

The remaining exercises examine the n-dimensional *Hurwitz zeta function*. Let $d > 0$ and define

$$\text{(9.3.5)} \qquad L_{\bar{a}}(s, d) := \sum_{\{i \mid a_i \neq 0\}} \sum_{n_i=0}^{\infty} \frac{\Pi\, s_i^{n_i}}{(\Sigma\, |a_i| n_i + d)^s}$$

where $s_i := \operatorname{sign}(a_i)$ and $\bar{a} := (a_1, a_2, \ldots, a_N)$. Thus

$$L_{-1,-1}(s,2) = \sum_{n,m=1}^{\infty} \frac{(-1)^{n+m}}{(n+m)^s}$$

and

$$L_{-1,2,3}(s,1) = \sum_{n,m,p=0}^{\infty} \frac{(-1)^n}{(n+2m+3p+1)^s} \, .$$

3. a) Show that

$$L_{\bar{a}}(s,d) = \Gamma^{-1}(s) \int_0^1 \frac{x^{d-1}(-\log x)^{s-1}\, dx}{\prod_{a_i \neq 0} (1 - s_i x^{a_i})} \, .$$

Hint: Take a Mellin transform. Then make a logarithmic variable change and sum the resultant series.

b) Let $L_{\bar{e}}(s,d) =: A_N(s,d)$ and $L_{-\bar{e}}(s,d) =: A_{-N}(s,d)$, where $\bar{e}$ is the vector $(1,1,\ldots,1)$ in $\mathbb{R}^N$. Show that for $d > 1$

$$\text{(9.3.6)} \qquad A_{\pm N}(s,d) = \frac{\mp 1}{N-1} [(d-1)A_{\pm(N-1)}(s, d-1) - A_{\pm(N-1)}(s-1, d-1)] \, .$$

Hint: Use integration by parts.

c) Combine integration by partial fractions and the recursion (9.3.6) to show that every sum of the form (9.3.5) factors into a linear combination of one-dimensional Hurwitz zeta functions (with coefficients depending on s).

4. Let $A_N(s) := A_{-N}(s,N)$ and $P_N(s) := A_N(s,N)$.

a) Show that

$$A_N(s) = A_{N-1}(s) - \frac{1}{N-1} A_{N-1}(s-1)$$

and

$$P_N(s) = \frac{1}{N-1} P_{N-1}(s-1) - P_{N-1}(s) \, .$$

b) Deduce that, for appropriate s,

i) $\displaystyle \sum_{m,n=1}^{\infty} \frac{(-1)^{m+n}}{(m+n)^s} = \alpha(s) - \alpha(s-1)$

ii) $\displaystyle \sum_{m,n=1}^{\infty} \frac{(-1)^{m+1}}{(m+n)^s} = \frac{1}{2}[\zeta(s) - \alpha(s)] = 2^{-s}\zeta(s)$

iii) $\displaystyle \sum_{m,n=1}^{\infty} \frac{1}{(m+n)^s} = \zeta(s-1) - \zeta(s).$

Thus

iv) $\displaystyle \sum_{-\infty}^{\infty}{}' \frac{(-1)^{m+n+1}}{(|m|+|n|)^s} = 4\alpha(s-1)$

v) $\displaystyle \sum_{-\infty}^{\infty}{}' \frac{1}{(|m|+|n|)^s} = 4\zeta(s-1).$

c) Show that

$$(N-1)!\,P_N(s) = \sum_{n=1}^{N} a_n^N \zeta(s-1+n)$$

where a_n^N are *Stirling numbers* of the first kind. Thus

$$P_4(s) = \tfrac{1}{6}\zeta(s-3) - \zeta(s-2) + \tfrac{11}{6}\zeta(s-1) - \zeta(s)$$

and

$$P_5(s) = \tfrac{1}{24}\zeta(s-4) - \tfrac{5}{12}\zeta(s-3) + \tfrac{35}{24}\zeta(s-2) - \tfrac{25}{12}\zeta(s-1) + \zeta(s) \, .$$

There is a similar formula for $A_N(s)$.

5. a) Show that

$$\sum_{-\infty}^{\infty}{}' \frac{(-1)^{n+m+k+1}}{(|n|+|m|+|k|)^s} = 2\alpha(s) + 4\alpha(s-2) \, .$$

b) Show that

$$\sum_{n,m=0}^{\infty} \frac{(-1)^{n+m}}{(2n+m+1)^s} = \left(\frac{1-2^{-s}}{2}\right)\alpha(s) + \frac{1}{2}\beta(s) \, .$$

c) Show that

$$\sum_{n,m=1}^{\infty} \frac{(-1)^{n+m}}{(3n+m)^s} = \frac{1}{3}[(2+3^{-s})\alpha(s) - \alpha(s-1) - L_{-3}(s,1)]$$

and so $L_{-1,-3}(1,4) = \dfrac{1}{3}\left[\dfrac{7}{3}\log 2 - \dfrac{\pi}{3\sqrt{3}} - \dfrac{1}{2}\right].$

6. Show that

$$\sum_{n,m,p=1}^{\infty} \frac{(-1)^{n+m+p+1}}{(n+2m+4p)^s} + \sum_{n=0}^{\infty} \frac{1}{(8n+7)^s} = 8^{-s}\zeta(s) \, .$$

Hint: $(1+x)(1+x^2)\cdots(1+x^{2^N-1}) = (1-x^{2^N})/(1-x)$.

9.4 *THE QUINTUPLE-PRODUCT IDENTITY*

Jacobi's triple-product identity has an elegant fivefold analogue due to Watson [29] and Gordon [61]. This is

$$(9.4.1)\quad \prod_{n=1}^{\infty}(1-q^n)(1-zq^n)(1-z^{-1}q^{n-1})(1-z^2q^{2n-1})(1-z^{-2}q^{2n-1})$$
$$=\sum_{m=-\infty}^{\infty}(z^{3m}-z^{-3m-1})q^{m(3m+1)/2}$$

valid for all complex z and q with $|q|<1$ and $z\neq 0$. The proof is left as an exercise. (See Exercise 1.)

If we divide both sides by $1-z^{-1}$ and let z tend to 1, we derive

$$\prod_{n=1}^{\infty}(1-q^n)^3(1-q^{2n-1})^2=\sum_{m=-\infty}^{\infty}(6m+1)q^{m(3m+1)/2}.$$

Now this yields

$$(9.4.2)\qquad \theta_4^2(q)=\frac{\Sigma_{m=-\infty}^{\infty}(6m+1)q^{m(3m+1)/2}}{\Sigma_{m=-\infty}^{\infty}(-1)^m q^{m(3m+1)/2}}$$

on using Euler's pentagonal formula (3.1.10) and (3.1.7). This can be used to establish a recurrence formula for $r_2(n)$, as in Ewell [82]. (See Exercise 4.)

Comments and Exercises

The identity, implicit in Ramanujan's work, was discovered by Watson [29] and rediscovered by Gordon [61]. Further extensions are discussed by Gordon. Other proofs abound in the literature.

1. Prove (9.4.1). As with the triple-product identity, it is easy to establish the formula (9.4.1) up to a constant relying on q alone. To evaluate the constant observe that when $z:=-1$, (9.4.1) reduces to Euler's pentagonal identity.

2. Show that (9.4.1) is equivalent to

$$\prod_{n=1}^{\infty}(1-q^{2n})(1-q^{2n-1}z)(1-q^{2n-1}z^{-1})(1-q^{4n-4}z^2)(1-q^{4n-4}z^{-2})$$
$$=\sum_{n=-\infty}^{\infty}q^{3n^2-2n}[(z^{3n}+z^{-3n})-(z^{3n-2}+z^{-(3n-2)})].$$

3. a) Let $q:=q^j$ and $z:=q^{-k}$ in (9.4.1) and deduce that

$$(9.4.3)\quad \prod_{n\in N(j,k)}(1-q^n)=\sum_{m=-\infty}^{\infty}q^{j(3m^2+m)/2}[q^{-3mk}-q^{(3m+1)k}]$$

where $N(j,k)$ consists of all integers congruent to $0, \pm k, j, j\pm k, j\pm 2k \pmod{2j}$ (repeated as appropriate).

b) Deduce that Euler's identity follows for $j:=4$ and $k:=1$. For $j:=3$ and $k:=1$ one gets

$$\prod_{n=1}^{\infty}(1-q^n)(1-q^{6n-5})(1-q^{6n-1})=g(q)-3qg(q^9)$$

where $g(q):=\Sigma_{n=0}^{\infty}q^{(n^2+n)/2}$. With $f(q):=\Pi_{n=1}^{\infty}(1-q^n)^{-1}$ this becomes a formula due to Ramanujan

$$\frac{f(q^2)f(q^3)}{f^2(q)f(q^6)}=g(q)-3qg(q^9).$$

c) Use $g(q)=f(q)/f^2(q^2)$ to obtain a functional equation for $f(q)$ (the partition function).

d) Use (9.4.3) with $j:=6$ and $k:=1$ to obtain

$$\frac{2f(q^2)f(q^3)f(q^{12})}{f(q)f(q^4)f^2(q^6)}=3\theta_3(q^9)-\theta_3(q).$$

Hence obtain a functional equation for θ_3. Thus note that $3\theta_3(q^9)=\theta_3(q)$ never has a solution. (Compare Section 4.7.)

4. a) Establish equation (9.4.2) and

$$\theta_4^2(q^{24})=\frac{\Sigma_{m=-\infty}^{\infty}(6m+1)q^{(6m+1)^2}}{\Sigma_{m=-\infty}^{\infty}(-1)^m q^{(6m+1)^2}}.$$

b) Use (9.4.2) to derive a recursion for $r_2(n)$.

c) Prove that

$$\prod_{n=1}^{\infty}(1-q^{2n})(1-q^{2n-1})^2(1-q^{4n})^2=\sum_{m=-\infty}^{\infty}(3m+1)q^{3m^2+2m}.$$

(9.4.4)

Hint: Use Exercise 2.

d) Show that

$$\sqrt{k'}=\frac{\theta_4(q)}{\theta_3(q)}=\frac{\Sigma_{n=-\infty}^{\infty}(3n+1)q^{(3n+2)n}}{\Sigma_{n=-\infty}^{\infty}(-1)^n(3n+1)q^{(3n+2)n}}$$

so that

$$\sqrt{k'} = \frac{\sum_{n=-\infty}^{\infty} (3n+1)q^{(3n+1)^2/3}}{\sum_{n=-\infty}^{\infty} (-1)^n(3n+1)q^{(3n+1)^2/3}}\,.$$

Observe that this is slightly faster to compute than the original theta series ratio.

e) Show that

$$\sqrt{k} = \frac{\theta_2(q)}{\theta_3(q)} = 2q^{1/4}\,\frac{\sum_{n=-\infty}^{\infty} (3n+1)q^{(3n+2)n}}{\sum_{n=-\infty}^{\infty} (6n+1)q^{(3n+1)n}}$$

so that

$$\sqrt{k} = \frac{\sum_{n=-\infty}^{\infty} (6n+2)q^{(6n+2)^2/12}}{\sum_{n=-\infty}^{\infty} (6n+1)q^{(6n+1)^2/12}}\,.$$

5. a) Show that

$$\sum_{i,j,k=-\infty}^{\infty} \frac{(-1)^{i+j+k}}{[24i^2+24j^2+(6k+1)^2]^s}$$

$$= \sum_{m=0}^{\infty}\left[\frac{1}{(6m+1)^{2s-1}} - \frac{1}{(6m+5)^{2s-1}}\right] = (1+2^{1-2s})L_{-3}(2s-1)\,.$$

b) Replace q by $-q$ in a) to express $L_{-24}(2s-1)$ as a lattice sum.

c) Combine (9.4.4) and (3.2.7) to prove that

$$L_{-3}(2s-1) = \sum \frac{(-1)^{i+j+k}}{[6(i+\frac{1}{4})^2 + 6(j+\frac{1}{4})^2 + 9(k+\frac{1}{6})^2]^s}\,.$$

Observe that at $s=\frac{1}{2}$ this equals $\frac{1}{3}$.

Gordon [61] also gives various congruences, like those given in Chapter 3 for the partition function. For example,

$$\frac{f(q^2)}{f(q)f(q^4)} =: \sum_{n=0}^{\infty} c_n q^n$$

has c_{3n+2} divisible by 3.

6. There is yet another remarkable identity due to Ramanujan, which includes both the triple-product and the q-binomial theorems. This is the ${}_1\Psi_1$ sum, whose derivation and uses are accessibly described in Askey [80]. In standard notation one writes

$$(9.4.5)\qquad \sum_{-\infty}^{\infty} \frac{(a;q)_n}{(b;q)_n}x^n = \frac{(ax;q)_\infty(q/ax;q)_\infty(q;q)_\infty(b/a;q)_\infty}{(x;q)_\infty(b/ax;q)_\infty(b;q)_\infty(q/a;q)_\infty}$$

where $(a;q)_\infty := \prod_{k=0}^{\infty}(1-aq^k)$ and $(a;q)_n := \dfrac{(a;q)_\infty}{(aq^n;q)_\infty}$.

This converges at least for $|q|<1$ and $|b/q|<|x|<1$.

a) Verify that the triple product is contained in (9.4.5).
Hint: Begin by setting $a := c^{-1}$, $x := cx$ and $b := 0$. Now let $c := 0$.

b) For $b := q$ (9.4.5) becomes the *q-binominal theorem*:

$$\sum_{n=0}^{\infty} \frac{(a;q)_n}{(q;q)_n}x^n = \frac{(ax;q)_\infty}{(x;q)_\infty}$$

valid for $|x|<1$ and $|q|<1$. Verify that Cauchy's binomial theorem is a special case. *Hint*: Begin by setting $a := q^{-2n}$.

c) Use the q-binomial theorem to express the limit mean of Example 8.4 as a Taylor series.

9.5. *QUINTIC AND SEPTIC MULTIPLIERS AND ITERATIONS*

In this section we discuss additional modular and multiplier identities and give a number of applications. Notations are as in Sections 4.6 and 4.7. References to entries are all to Chapter 19 in Ramanujan's Second Notebook (Berndt [Pr]).

Proposition 9.2

(a)

$$(9.5.1)\qquad 5M_5 = 1 + 2G_{25n}/G_n^5$$

$$(9.5.2)\qquad 1/M_5 = 1 + 2G_n/G_{25n}^5$$

$$(9.5.3)\qquad 5M_5 + 1/M_5 = 2\{2 + kl + k'l'\}\,.$$

(b) Let $1/(2t+1) := M_5$. Then

$$(9.5.4)\qquad 1-2l^2 = M_5^2(1-11t-t^2)\sqrt{(1+t^2)M_5}$$

$$(9.5.5)\qquad 1-2k^2 = (1+t-t^2)\sqrt{(1+t^2)M_5}\,.$$

Proof.

(*a*) These are given in Entry 13. Berndt [Pr] provides proofs which may also be deduced from (4.1.20).

(*b*) These may similarly be found in Entry 14. □

We will write, as in Section 4.7,

$$M_p(n) := M_p(k_n, k_{p^2n})\,.$$

Ramanujan also gives the following beautiful counterpart to Theorem 4.11 (Entry 12(iii)).

Theorem 9.2

$$5\,\frac{\theta_3(q^{25})}{\theta_3(q)} = 1 + r_1^{1/5} + r_2^{1/5} \tag{9.5.6}$$

where for $i = 1$ or 2

$$r_i := \tfrac{1}{2}x(y \pm \sqrt{y^2 - 4x^3}) \tag{9.5.7}$$

and

$$x := 5\,\frac{\theta_3^2(q^5)}{\theta_3^2(q)} - 1, \quad y := (x-1)^2 + 7\,. \tag{9.5.8}$$

This provides a solvable update for M_5 despite the nonsolvable nature of W_5 (See Exercise 8 of Section 4.5). Indeed with $m_n := 5M_5(r5^{2n})$ we have

$$m_{n+1} = (1 + r_1^{1/5} + r_2^{1/5})^2/m_n \tag{9.5.9}$$

with $x := m_n - 1$, y and r_i as above.

If we combine (9.5.9) with the following formula for ε_5 we obtain a remarkably simple solvable 5th-order iteration for π.

Proposition 9.3

If $r > 0$ and $s(r) := M_5^{-1}(r)$ then

$$\alpha(25r) = s^2(r)\alpha(r) - \sqrt{r}\left\{\frac{s^2(r) - 5}{2} + \sqrt{s(r)(s^2(r) - 2s(r) + 5)}\right\}. \tag{9.5.10}$$

Proof.

We begin with ε_5, as given by (5.2.13), and the explicit formula for R_5. We use Proposition 9.2(a) to rewrite $s(r)R_5$ and 9.2(b) for the terms involving l^2 and k^2. This leads reasonably directly to

$$\varepsilon_5 = \frac{s^2(r) - 5}{2} + \sqrt{s(r)(s^2(r) - 2s(r) + 5)}\,.$$

Now (5.2.14) becomes (9.5.10). (Exercise 2.) □

The identical manipulations to those in Example 5.3 immediately yield $\alpha(5) = \frac{1}{2}\{\sqrt{5} - \sqrt{2(\sqrt{5} - 1)}\}$.

We next list several similar identities for M_7.

Proposition 9.4

(a)

$$49M_7^2 = \frac{l}{k} + \frac{l'}{k'} - \frac{ll'}{kk'} - 8\left(\frac{ll'}{kk'}\right)^{2/3} \tag{9.5.11}$$

$$1/M_7^2 = \frac{k}{l} + \frac{k'}{l'} - \frac{kk'}{ll'} - 8\left(\frac{kk'}{ll'}\right)^{2/3}. \tag{9.5.12}$$

(b) Let $t := (kl)^{1/4}$. Then

$$7M_7 - 1/M_7 = 6 - 16t + 12t^2 - 8t^3\,. \tag{9.5.13}$$

Proof. These are to be found in Entry 19. □

From (9.5.13) and (4.6.7) we may establish that for $r > 0$ and $s(r) := M_7^{-1}(r)$

$$\alpha(49r) = s^2(r)\alpha(r) - \sqrt{r}\left\{\frac{s^2(r) - 7}{2} + s(r)(4t^2 - 4t + 3)\right\}, \tag{9.5.14}$$

where $t^4 = kl$. (See Exercise 3.)

Ramanujan does not give a septic analogue to Theorem 9.2. He does, however, give quintic and septic updates for the *eta-multiplier*. Let η be given by (3.2.9) and (3.2.11). Let

$$N_p := \frac{\eta^2(q)}{\eta^2(q^{1/p})} \tag{9.5.15}$$

so that N_p corresponds to M_p. This is the *eta-multiplier of order p*. Now (3.2.15) can be written as

$$kk'M_p^3 = ll'N_p^3 \quad \text{or} \quad M_p = N_p\left(\frac{ll'}{kk'}\right)^{1/3}, \tag{9.5.16}$$

where $W_p(l^2, k^2) = 0$.

Theorem 9.3

(a)

$$N_2^6 = \frac{M_2(1 - M_2)}{4(2M_2 - 1)} \tag{9.5.17}$$

(9.5.18) $$N_3^3 = \frac{M_3(1-M_3^2)}{9M_3^2-1}$$

(9.5.19) $$N_5^3 = \frac{M_5(1-M_5)^2}{(5M_5-1)^2} .$$

(b)

(9.5.20) $$(49M_7^2-1)N_7^3 - (8M_7)N_7^2 + (8M_7^2)N_7 + M_7(M_7^2-1) = 0 .$$

Proof.

(*a*) In each case one combines (9.5.16) with appropriate multiplier equations. For $p := 5$ use (9.5.1) and (9.5.2). For $p := 3$ use the identities preceding equation (4.7.9). (The details are left as Exercise 6a).)

(*b*) We use (9.5.11) and (9.5.12) to write

$$ll'M_7^{-2}(1+8N_7^2) = kl' + lk' - kk'$$

and

$$kk'M_7^2(49 + 8/N_7^2) = kl' + lk' - ll' .$$

We now subtract one from the other and divide by ll'. □

We finish the section by listing Ramanujan's updates for N_5 and N_7. Entry 12(i) can be recast as

(9.5.21) $$5N_5(q^5) = (\mu^{1/5} + \nu^{1/5} - 1)^2/(5N_5(q))$$

where μ and υ are the solutions to

$$\mu\nu = -1 , \quad \mu + \nu = 11 + (5N_5(q))^3 .$$

Entry 18(ii) becomes

(9.5.22) $$7N_7(q^7) := (\mu^{1/7} + \nu^{1/7} + \omega^{1/7} - 1)^2/(7N_7(q))$$

where μ, ν and ω are the roots of

$$x^3 - ax^2 - bx + 1 = 0$$

and a and b are given by

$$a := 57 + 14[7N_7(q)]^2 + [7N_7(q)]^4$$

$$b := 289 + 126[7N_7(q)]^2 + 19[7N_7(q)]^4 + [7N_7(q)]^6 .$$

Theorem 9.2 gives $\theta_3(q^{25})$ solvably in terms of $\theta_3(q^5)$ and $\theta_3(q)$. Likewise (9.5.22) gives $\theta_3(q^{49})$ solvably in terms of $\theta_3(q^7)$ and $\theta_3(q)$. Thus $\theta_4(q) = \theta_3(-q)$ is similarly solvable and since $k = \theta_4^2/\theta_3^2$ and j is solvable in k we see that for f any of θ_4, k, g, G or J, $f(q^p)$ is solvable over $\mathbb{Q}(f(q), f(q^{1/p}))$; for $p := 5$ and for $p := 7$. In view of the nonsolvability of the quintic or septic modular equations for λ (and hence k and j), this is at first surprising. What is happening is that the Galois group for F_p, $p \geq 5$ and prime, is a nonsolvable group of order $(p-1)p(p+1)/2$. However $j(q^{1/p})$ is a root of F_p and, since F_p is irreducible, it is of order $p+1$. Thus the splitting field for F_p over $\mathbb{Q}_p(j(q), j(q^{1/p}))$ has order dividing $p(p-1)/2$. For $p := 3, 5, 7$, and 11, $(p-1)/2$ is prime and the corresponding group is obviously solvable. For $p := 7$, for example, we expect seventh roots of cube roots to comprise the solution $((p-1)/2 = 3)$. This is consistent with equations (9.5.22) and (9.5.20).

Comments and Exercises

Knowing that a solution exists and exhibiting it, particularly in simple form, can be very different matters. The components of the quintic and septic algorithms for π are far less complicated than one might initially expect. Both can be packaged very elegantly. (See Exercises 2 and 7, and Borwein and Borwein [Pr].)

1. a) Combine (9.5.1) and (9.5.2) to obtain Schlafli's form of the quintic modular equation.

b) Compute that

i) $M_5^{-1}(1/5) = \sqrt{5}$

ii) $M_5^{-1}(1) = 5(\sqrt{5}-2)$

iii) $M_5^{-1}(3/5) = \dfrac{(5-\sqrt{5})}{2}$

iv) $M_5^{-1}(2/5) = \sqrt{5}(\sqrt{5}+2)(\sqrt{2}-1)^2$.

c) Find closed forms for $M_5^{-1}(n)$ for $n := 1, 5, 9$, and 25.

d) Use $G_{85} = [(\sqrt{5}+1)/2][(9+\sqrt{85})/2]^{1/4}$ and the conjugate nature of $G_{17/5}$ to compute $5M_5(\frac{17}{5})$. Use Theorem 5.4 to compute $\sigma(85)$.

2. a) Verify the formula (9.5.10) for $\alpha(25r)$.

b) Obtain closed forms for $\alpha(n)$ $n = 25$, 125, 625, 225, and 1225 (Ramanujan [14] gives G_{1225}).

c) Observe that Exercise 1b) (9.5.9) and (9.5.10) combine to give several explicit iterations for π. For example, we may begin with $r := 1$, $\alpha(1) = \frac{1}{2}$, $s(1) = 5(\sqrt{5}-2)$.

d) Use Theorem 9.2 to compute G_{625n} in terms of G_n and G_{25n}.

3. a) Show that (9.5.14) holds and that

$$\varepsilon_7 := \frac{s^2(r) + 2s(r) - 7}{2} + 2s(r)\{\sqrt{lk} + \sqrt{l'k'}\}.$$

b) Compute the corresponding updates for $\delta(25r)$ and $\delta(49r)$. In particular

$$\delta(49) = M_7^{-1}(1)\{1 + 2\sqrt{kl} + 2\sqrt{k'l'}\}.$$

c) Verify $\alpha(7)$.
d) Establish that R_5 and R_7 are as given in Table 5.1.

4. Ramanujan also gives (Entry 19)

$$M_7^{-1} = \frac{1 - 4\left\{\dfrac{(kk')^7}{ll'}\right\}^{1/12}}{(k'l')^{1/4} - (kl)^{1/4}}$$

$$7M_7 = \frac{1 - 4\left\{\dfrac{(ll')^7}{kk'}\right\}^{1/12}}{(kl)^{1/4} - (k'l')^{1/4}}.$$

a) Thus show

$$7M_7^2 = \left(\frac{G_{49n}}{G_n}\right)^7 \frac{G_n^7 - 2\sqrt{2}G_{49n}}{2\sqrt{2}G_n - G_{49n}^7}.$$

b) Compute $M_7(\frac{3}{7})$ and $M_7(\frac{15}{7})$.

5. Ramanujan in his letters (Hardy [40] p. 353) gives the following beautiful hybrid identity. Let

$$Q := \left(\frac{G_n G_{225n}}{G_{9n} G_{25n}}\right)^{3/2}, \qquad P := (G_n G_{9n} G_{25n} G_{225n})^{1/2}.$$

Then

$$\sqrt{2}\left(P + \frac{1}{P}\right) = Q + \frac{1}{Q}.$$

a) Verify that $G_{15}^3 = \dfrac{8^{1/4}(\sqrt{5}+1)}{2}$ and $G_{5/3}^3 = \dfrac{8^{-1/4}(\sqrt{5}+1)}{2}$.

6. a) Establish the eta-multiplier formulae of Theorem 9.3a) and b).

b) Show that $N_p(k_p', k_p) = \dfrac{1}{\sqrt{p}}$.

c) Show that

$$49M_7^2 = \tfrac{1}{2}(P(y) + \sqrt{P^2(y) + 196y^3})$$
$$1/M_7^2 = \tfrac{1}{2}(P(x) + \sqrt{P^2(x) + 196x^3})$$

where $x := (kk'/ll')^{1/3}$, $y := (ll'/kk')^{1/3}$ and

$$P(x) := 1 + 8x - 8x^2 - x^3.$$

d) Prove that if $x := \sqrt{M_{13}}$ and $y := \sqrt{N_{13}}$

$$(1 - 13x^2)y^3 + (4x)y^2 - (4x^2)y + x(1 - x^2) = 0.$$

Hint: Use (4.6.8).

7. Combine (9.5.20) and (9.5.22) to produce a solvable update for $m_n := 7M_7(r7^{2n})$; and so a solvable 7th-order iteration for π.

8. Ramanujan's letters also contain the modular equations of degree 5 for $K_{1/4}$ and $K_{1/6}$. (See Section 5.5.) For $K_{1/6}$ one has

$$(lk)^{2/3} + (l'k')^{2/3} + 3(ll'kk')^{1/3} = 1$$

and for $K_{1/4}$ one has

$$lk + l'k' + 8(ll'kk')^{1/3}\{(lk)^{1/3} + (l'k')^{1/3}\} = 1.$$

a) Verify that, in the notation of (5.5.34),

$$G_{1/6}^{-12}(5) = \frac{2}{5\sqrt{5}}.$$

b) Similarly

$$G_{1/4}^{-12}(5) = \frac{1}{9}.$$

Hint: The appropriate pth-order modular transformation for K_s sends $1 =: \lambda_s^*(n)$ to $k := \lambda_s^*(p^2 n)$.

Chapter Ten

Other Approaches to the Elementary Functions

Abstract. *We examine some of the standard polynomial and rational approximations to elementary functions, particularly to exp and log. We discuss methods for reducing the complexity of calculating these functions based on accelerating the evaluation of the approximants. While these methods are usually less than optimal, they are of more general application than those of Chapters 6 and 7.*

10.1 CLASSICAL APPROXIMATIONS

We commence with an analysis of the standard approximations to exp on a disk $D_\delta := \{|z| \le \delta\}$. The notations we will require are as follows. Let P_n denote the algebraic polynomials of degree at most n with real coefficients. Let $\|f\|_A$ denote the supremum norm of a continuous function f on the set A, that is,

(10.1.1) $$\|f\|_A := \sup_{x\in A} |f(x)|\,.$$

For a continuous f on an infinite compact set $A \subset \mathbb{C}$, let

(10.1.2) $$E_n(f, A) := \min_{p\in P_n} \|f - p\|_A$$

and let

(10.1.3) $$R_n(f, A) := R_n(f) = \min_{p,q\in P_n} \|f - p/q\|_A\,.$$

These quantities are, respectively, the error in best uniform polynomial and

best uniform rational approximations. The existence of the best approximants is fairly straightforward and is left as Exercise 2.

The most commonly used polynomial approximations to exp are undoubtedly the partial sums of the Taylor series. This is reasonable since in any neighbourhood of zero the partial sums are asymptotically optimal. (See also Exercise 3.)

Theorem 10.1

(*a*) $$\left\|e^z - \sum_{i=0}^{n} \frac{z^i}{i!}\right\|_{D_1} \le \frac{1}{(n+1)!}\left(1 + \frac{2}{n+1}\right).$$

(*b*) If $p \in P_n$, then

$$\|e^z - p(z)\|_{D_1} \ge \frac{1}{(n+1)!}\left(1 - \frac{2}{n+1}\right).$$

Proof. Part (*a*) follows from the estimate

$$\sum_{i=n+1}^{\infty} \frac{1}{i!} \le \frac{1}{(n+1)!}\left[1 + \frac{1}{n+2}\left(1 + \frac{1}{n+3} + \frac{1}{(n+3)(n+4)} + \cdots\right)\right].$$

For part (*b*) we observe that if

$$\|e^z - p(z)\|_{D_1} < \min_{|z|=1} |e^z - s_n(z)|$$

where s_n is the nth partial sum to exp at zero, then by Rouché's theorem

$$p(z) - s_n(z) \qquad \text{and} \qquad e^z - s_n(z)$$

have the same number of zeros (counting multiplicity) in D_1. As $e^z - s_n(z)$ has a zero of order $n+1$ at zero, we deduce the contradiction that $p \equiv s_n$. To finish the proof we need only observe that

$$\min_{|z|=1} |e^z - s_n(z)| > \frac{1}{(n+1)!}\left(1 - \frac{2}{n+1}\right). \quad \square$$

We now turn to the Padé approximants to exp. These are rational approximations that are a natural extension of the Taylor approximants. We define

(10.1.4) $$r_{m,n}(z) := \frac{\int_0^\infty t^n(t+z)^m e^{-t}\,dt}{\int_0^\infty (t-z)^n t^m e^{-t}\,dt}$$

and observe that $r_{m,n}$ is a rational function of z with numerator of degree m and denominator of degree n. In closed form, (10.1.5) $$r_{m,n}(z)=\sum_{v=0}^{m}\frac{\binom{m}{v}}{\binom{n+m}{v}}\frac{z^v}{v!}\Big/\sum_{v=0}^{n}\frac{\binom{n}{v}}{\binom{m+n}{v}}\frac{(-z)^v}{v!}\,.$$

Theorem 10.2

(*a*) $$\|e^z-r_{n,n}(z)\|_{D_1}\le\frac{8(n!)(n!)}{(2n)!(2n+1)!}\,.$$

(*b*) If $p, q\in P_n$, then

$$\left\|e^z-\frac{p(z)}{q(z)}\right\|_{D_1}\ge\frac{(n!)(n!)}{8(2n)!(2n+1)!}\,.$$

Proof. Let

(10.1.6) $$q_n(z):=(2n)!\sum_{v=0}^{n}\frac{\binom{n}{v}(-z)^v}{\binom{2n}{v}v!}=\int_0^\infty (t-z)^n t^n e^{-t}\,dt\,.$$

Then

(10.1.7) $$\begin{aligned}q_n(z)[e^z-r_{n,n}(z)]&=\int_0^\infty (t-z)^n t^n e^{z-t}\,dt-\int_0^\infty t^n(t+z)^n e^{-t}\,dt\\&=\int_0^z (t-z)^n t^n e^{z-t}\,dt\\&=z^{2n+1}\int_0^1 (u-1)^n u^n e^{(1-u)z}\,du\,.\end{aligned}$$

Now from (10.1.6), for $|z|\le 1$,

(10.1.8) $$\begin{aligned}|q_n(z)|&\ge n!\left[\frac{(2n)!}{n!}-\frac{(2n-1)!}{(n-1)!}-\frac{(2n-2)!}{2!(n-2)!}-\cdots\right]\\&\ge(2n)!\left(1-\frac{1}{2}-\frac{1}{2^2 2!}-\cdots\right)\\&\ge(2n)!(2-\sqrt{e})\,.\end{aligned}$$

Since

(10.1.9) $$\int_0^1 (1-u)^n u^n\,du=\beta(n+1,n+1)=\frac{n!n!}{(2n+1)!}$$

we have from (10.1.7) and (10.1.8),

(10.1.10) $$\|e^z-r_{n,n}(z)\|_{D_1}\le\frac{e}{2-\sqrt{e}}\,\frac{n!n!}{(2n)!(2n+1)!}\,.$$

Part (*b*) requires showing that for $|z|=1$,

(10.1.11) $$|e|^z-r_{n,n}(z)|>\frac{n!n!}{8(2n)!(2n+1)!}$$

which follows from the estimates (Exercise 5)

(10.1.12) $$\left|\int_0^1 (u-1)^n u^n e^{(1-u)z}\,du\right|\ge\frac{1}{4}\,\frac{n!n!}{(2n+1)!}$$

and

(10.1.13) $$|q_n(z)|\le(2n)!\sqrt{e}\,.$$

The rest of the argument is analogous to part (*b*) of Theorem 10.1. If there were a rational function p/q satisfying (*b*) with the inequality strictly reversed, then by (10.1.11) and Rouché's theorem,

$$p/q-r_{n,n}\qquad\text{and}\qquad e^z-r_{n,n}$$

would both have the same number of zeros, and from (10.1.7) we would deduce that $p/q-r_{n,n}$ has at least $2n+1$ zeros and hence is identically zero. □

The fact that $r_{n,n}$ is the Padé approximant is a consequence of (10.1.7), which shows that

$$e^z-r_{n,n}(z)=O(z^{2n+1})\qquad\text{as}\qquad z\to 0\,.$$

In general the (m, n) *Padé approximant* to an f (analytic at zero) is the unique rational function $r=p/q$, where $p\in P_m$ and $q\in P_n$, which satisfies

$$f(z)-p(z)/q(z)=O(z^h)$$

where h (in nondegenerate cases $h=m+n+1$) is as large as possible. For $n=0$ this defines the nth Taylor polynomial.

The following is a partial list of the standard series and continued fraction expansions for exp and log.

$$e^z = \sum_{n=0}^{\infty} \frac{z^n}{n!} \tag{10.1.14}$$

$$e^z = 1 + \frac{2z}{2 - z + 2z^2 \sum_{n=1}^{\infty} [1/(z^2 + (2\pi n)^2)]} \tag{10.1.15}$$

$$e^z = 1 + \frac{z}{1-}\,\frac{z}{2+}\,\frac{z}{3-}\,\frac{z}{2+}\,\frac{z}{5-}\,\frac{z}{2+}\,\frac{z}{7-}\cdots \tag{10.1.16}$$

$$\lim_{n\to\infty} \left(1 + \frac{z}{n}\right)^n = e^z \tag{10.1.17}$$

$$\log(1+z) = \sum_{n=1}^{\infty} \frac{(-1)^{n+1} z^n}{n} \qquad |z| \le 1, \quad z \ne -1 \tag{10.1.18}$$

$$\log(z) = 2\left[\left(\frac{z-1}{z+1}\right) + \frac{1}{3}\left(\frac{z-1}{z+1}\right)^3 + \frac{1}{5}\left(\frac{z-1}{z+1}\right)^5 + \cdots\right] \qquad \operatorname{re}(z) > 0, \tag{10.1.19}$$

$$\log\left(\frac{z+1}{z-1}\right) = 2\left(\frac{1}{z} + \frac{1}{3z^3} + \frac{1}{5z^5} + \cdots\right) \qquad |z| \ge 1, \quad z \ne \pm 1 \tag{10.1.20}$$

$$\log(1+z) = \frac{z}{1+}\,\frac{z}{2+}\,\frac{z}{3+}\,\frac{4z}{4+}\,\frac{4z}{5+}\,\frac{9z}{6+}\,\frac{9z}{7+}\cdots \qquad z \notin (-\infty, -1] \tag{10.1.21}$$

$$\lim_{\delta \downarrow 0} \frac{z^\delta - 1}{\delta} = \log z\,. \tag{10.1.22}$$

Comments and Exercises

Padé approximants derive their name from H. Padé, a student of Hermite, who was one of the first to systematically study such approximations at the end of the last century. The theory of Padé approximation may be pursued in Baker and Graves-Morris [81]. The convergence theory for Padé approximants is far more complicated than the analogous well-known theory for Taylor series. (See Exercise 9.) Except in special cases, such as exp or functions given by Stieltjes transforms $[\int d\alpha(t)/(x+t)]$, analysis of region or rates of convergence is only partially understood. Theorem 10.2 can be sharpened to show that

$$R_n(e^z, D_1) \sim \frac{n!n!}{(2n)!(2n+1)!}$$

using Padé approximants centered at $z := 1/(2n+1)$. This is due to Trefethen [84]. (See Exercise 10.) The discussion of the approximations of exp follows Newman [79], as do Exercises 7 and 8. These exercises illustrate the different rates of convergence on disks and intervals. Exercise 8 is the $n = m$ case of a conjecture of Meinardus, namely, that

$$R_{n,m}(e^x, [-1, 1]) = \left[\frac{n!m!}{2^{n+m}(n+m+1)!(n+m)!}\right][1 + o(1)]$$

as $n + m \to \infty$. This conjecture has been resolved recently by Braess [84]. (See also Nemeth [77].)

For further discussion of the material of this section the reader is referred to Cheney [66] or Newman [79]. The various expansions may be found in Abramowitz and Stegun [64].

In Section 11.3 we will use the Padé approximant to exp to derive a precise irrationality measure for e.

1. (*Lagrange interpolation formula*) Given $n+1$ points in the plane, (z_i, w_i), $i = 0, \ldots, n$, so that $z_i \ne z_j$ for $i \ne j$, show that there exists a unique $p \in P_n$ so that

$$p(z_i) = w_i \qquad i = 0, \ldots, n\,.$$

Show that

$$p(z) = \sum_{i=0}^{n} w_i l_i(z)$$

where

$$l_i(z) := \prod_{\substack{k=0\\k\ne i}}^{n} \frac{z - z_k}{z_i - z_k}\,.$$

2. (*Existence of best approximants*) Prove that E_n and R_n are well defined, that is, show that the min is achieved in (10.1.2) and (10.1.3). *Hint*: A uniformly bounded sequence of polynomials, all of degree n has a uniformly convergent subsequence whose limit is a polynomial of degree at most n.

3. a) Suppose that f is entire and that s_n is the nth partial sum of f at zero. Show that

$$\limsup_{n\to\infty} \frac{E_n(f, D_1)}{\|f - s_n\|_{D_1}} = 1\,.$$

Hint: Show that if $f(z) =: \sum_{i=0}^{\infty} a_i z^i$, then for infinitely many m,

$$|a_m|(1-\varepsilon) \le \left|\sum_{i=m}^{\infty} a_i z^i\right| \le |a_m|(1+\varepsilon) \qquad |z| = 1 .$$

Now use the arguments of Theorem 10.1.

b) Suppose f is analytic in a neighbourhood of zero. For fixed n show that

$$\lim_{\delta \downarrow 0} \frac{E_n(f, D_\delta)}{\|f - s_n\|_{D_\delta}} = 1 .$$

Part a) illustrates that the Taylor approximants behave globally like best polynomial approximants to entire functions on disks. The story is different on different shaped regions. Part b) shows that locally the Taylor approximants are always optimal.

4. Prove that (10.1.4) has the representation (10.1.5).

5. Establish the estimates (10.1.12) and (10.1.13).

6. Establish the expansions (10.1.14) to (10.1.22).

7. (*Polynomial approximation to exp on* $[-1, 1]$) Let s_n be the nth partial sum of exp at zero.

a) Show that if $p(z)$ is a polynomial of degree n, then $p(z)p(1/z)$ is a polynomial of degree n in the variable $z + 1/z$.

b) If x is the real part of z, where $|z| = 1$, then $e^x = e^{z/2}e^{\bar{z}/2} = e^{z/2}e^{1/2z}$. On $|z| = 1$ approximate $e^{z/2}$ by $s_n(z/2)$ and approximate $e^{1/2z}$ by $s_n(1/2z)$ and estimate the errors.

c) Use part a) to construct polynomial approximations to exp that satisfy

$$E_n(e^x, [-1, 1]) \le \frac{e^{1/2} + o(1)}{2^n(n+1)!} .$$

Note the approximation is

$$e^x \sim \sum_{i=0}^{n} \frac{z^i}{i!2^i} \sum_{i=0}^{n} \frac{z^{-i}}{i!2^i} \qquad z := x + iy .$$

d) Modify part c) to show that

$$E_n(e^x, [-1, 1]) \le \frac{1 + o(1)}{2^n(n+1)!} .$$

(This is in fact asymptotically optimal.) *Hint*: Consider the method with approximation centered at $1/n$.

8. (*Rational approximation to exp on* $[-1, 1]$) Show that

$$R_n(e^x, [-1, 1]) \le \frac{8}{4^n} \frac{n!n!}{(2n)!(2n+1)!} .$$

Hint: Proceed as in 7). First observe that Exercise 7a) holds for rational functions of degree n. The approximation is given by

$$e^x - r_{n,n}\left(\frac{z}{2}\right) r_{n,n}\left(\frac{1}{2z}\right)$$

where $|z| = 1$ and $z := x + iy$. Use estimates like those in the proof of Theorem 10.2 to prove the result.

9. The $(n, 1)$ Padé approximant p_n to $f := \sum_{i=0}^{\infty} a_i z^i$ has denominator $a_{n+1}z - a_n$ and, provided $a_n \ne 0$, satisfies

$$p_n - f = O(z^{n+2}) .$$

a) Show that if f is entire, then there is a subsequence of $\{p_n\}$ that converges to f uniformly on any given compact subset of $\mathbb{C}$.

b) Show that there exists an entire function so that the full sequence $\{p_n\}$ does not converge uniformly on any open set in $\mathbb{C}$.
Hint: Show that the poles of the p_n can be dense in $\mathbb{C}$.

Exercise 9, due to Beardon and Perron, illuminates some of the problems inherent in uniform convergence questions for Padé approximants. It was conjectured that subsequential convergence holds for the sequence of (m, k) Padé approximants (k fixed) and for the sequence of (m, m) Padé approximants. Much of the conjecture concerning convergence along rows (k fixed) was recently settled by Buslaev, Gonchar, and Suetin [84]. They show, for example, that if f is entire, some subsequence of the (m, k) Padé approximants (k fixed) converges uniformly to f on compact subsets of $\mathbb{C}$. These conjectures, due variously to Baker, Gammel, Graves-Morris, Wills, and others are discussed in Baker and Graves-Morris [81]. A more complete convergence theory is available if one is prepared to settle for weaker types of convergence, for example, convergence in measure.

10. (*More on the Padé approximants to exp*) Let

$$p_{m,n}(z) := \int_0^{\infty} t^n (t+z)^m e^{-t}\, dt$$

$$q_{m,n}(z) := \int_0^{\infty} (t-z)^n t^m e^{-t}\, dt .$$

a) Show, as in the proof of Theorem 10.2, that

$$q_{m,n}(z)e^z - p_{m,n}(z) = z^{m+n+1} \int_0^1 (u-1)^n u^m e^{(1-u)z}\, du .$$

b) Show that, as $m + n \to \infty$,

$$q_{m,n}(z)e^z - p_{m,n}(z) = \frac{(-1)^n m!n!}{(m+n+1)!} e^{nz/(m+n)} z^{m+n+1} [1 + o(1)] .$$

Hint: Observe that $(u-1)^n u^m$ is essentially a "spike" at $u := m/(m+n)$ and that

$$\int_0^1 (u-1)^n u^m\, du = \frac{(-1)^n m!n!}{(m+n+1)!} .$$

c) Show that

$$p_{m,n}(z) := \sum_{k=0}^{m} \frac{m!(n+m-k)!}{(m-k)!k!} z^k$$

$$q_{m,n}(z) := \sum_{k=0}^{n} \frac{n!(n+m-k)!}{(n-k)!k!} (-1)^k z^k .$$

Recall that $\int_0^\infty t^n e^{-t}\, dt = n!$

d) Show that

$$P_{m,n} := \frac{p_{m,n}}{n!} \quad \text{and} \quad Q_{m,n} := \frac{q_{m,n}}{m!}$$

are polynomials with integer coefficients of degree m and n, respectively.

e) Show that, as $n, m \to \infty$,

$$p_{m,n}(z) = (n+m)!\, e^{[m/(n+m)]z} [1 + o(1)]$$

and

$$q_{m,n}(z) = (n+m)!\, e^{-[n/(n+m)]z} [1 + o(1)] .$$

The convergence is uniform on compact subsets.
Hint: Examine the coefficients of $p_{m,n}(z)/(n+m)!$

f) Show that, as $m, n \to \infty$,

$$e^z - \frac{p_{m,n}(z)}{q_{m,n}(z)} = \frac{(-1)^n m!n!}{(m+n)!(m+n+1)!} e^{[2n/(m+n)]z} z^{m+n+1} [1 + o(1)] .$$

The convergence is uniform on compact subsets that avoid any

zeros of the denominator sequence. Observe that, by e), only finitely many of these zeros lie in any compact set. Further details may be found in Trefethen [84] or Braess [84].

g) Show that

$$R_n(e^z, D_\rho) = \frac{n!n!\rho^{2n+1}}{2n!(2n+1)!} [1 + o(1)] .$$

Hint: Consider the Padé approximant centered at $2\rho^2/(2n+1)$. That is, replace z by $z - 2\rho^2/(2n+1)$ in parts e) and f). This gives the upper bound. Use Rouché's theorem, as in the proof of Theorem 10.2, to derive the lower estimate.

11. (*On the main diagonal Padé approximants to log*)

a) Suppose S_n and T_n are polynomials of degree n and suppose that

$$T_n(x) \log x - S_n(x) = O(1-x)^{2n+1} .$$

Show that, if $T_n(x) := t_0 + t_1 x + \cdots + t_n x^n$, then

$$[T_n(x) \log x]^{(n+1)} = \frac{(-1)^n n!}{x^{n+1}} \sum_{j=0}^{n} \frac{(-1)^j t_j x^j}{\binom{n}{j}}$$

and hence

$$\frac{x^{n+1}[T_n(x)\log x]^{(n+1)}}{(-1)^n n!} = \sum_{j=0}^{n} \frac{(-1)^j t_j x^j}{\binom{n}{j}} = (-1)^n t_n (x-1)^n .$$

b) Show that

$$T_n(x) = \sum_{k=0}^{n} \binom{n}{k}\binom{n}{k} x^k$$

if we normalize so that $t_n := 1$. [This is the denominator of the (n, n) Padé approximant to log at the point 1.] Observe that T_n is of degree n and has integral coefficients.

c) Show (with the above normalization, $t_n := 1$) that $d_n \cdot S_n$ has integer coefficients, where $d_n := \mathrm{LCM}(1, \ldots, n)$.

d) Let

$$\mathscr{E}_n(x) := \log x - \frac{S_n(x)}{T_n(x)} .$$

Show that

$$\mathscr{E}_n(x) := \int_1^x \frac{(1-u)^{2n}}{uT_n^2(u)}\, du .$$

Hint: Observe that $\mathscr{E}_n := O(1-x)^{2n+1}$. Now differentiate to get

$$\dot{\mathscr{E}}_n(x) = \frac{1}{x} - \frac{\dot{S}_n T_n - \dot{T}_n S_n}{T_n^2} = O(1-x)^{2n}.$$

Thus

$$xT_n^2(x)\dot{\mathscr{E}}_n(x) = T_n^2 - x(\dot{S}_n T_n - \dot{T}_n S_n) = O(1-x)^{2n}.$$

Since the middle term is a polynomial of degree $2n$ with lead coefficient 1, we must have

$$xT_n^2(x)\dot{\mathscr{E}}_n(x) = (1-x)^{2n}.$$

Show that

$$\mathscr{E}_n(x) = \frac{-\Sigma_{k=n}^{\infty}[k!k!/[(k+n+1)!(k-n)!]](1-x)^{n+k+1}}{\Sigma_{i=0}^{n}\binom{n}{i}\binom{n}{i}x^i}.$$

e) Show that

$$T_n(1) = \binom{2n}{n}$$

and that for $x \geq 0$,

$$\frac{(1+\sqrt{x})^{2n}}{2(n+1)} \leq T_n(x) \leq (1+\sqrt{x})^{2n}.$$

f) Show that, for $x \in (1-\delta, 1+\delta)$,

$$\frac{c_\delta}{n}\left(\frac{1-\sqrt{x}}{1+\sqrt{x}}\right)^{2n} \leq |\mathscr{E}_n(x)| \leq nd_\delta\left(\frac{1-\sqrt{x}}{1+\sqrt{x}}\right)^{2n}$$

where $c_\delta > 0$ and $d_\delta > 0$ depend only on δ, $0 < \delta < 1$.

10.2 *REDUCED COMPLEXITY METHODS*

We are primarily concerned with methods that accelerate the evaluation of the elementary function by reducing the complexity of evaluating one of the standard approximants. Most of the approximants listed in the previous section evaluated by usual methods (such as, Horner's rule) provide between $O(n)$ and $O(n \log n)$ digits for n arithmetic operations. The slight difference comes from the more rapid convergence of the Taylor polynomials for exp

than those for log. (See Exercise 1.) We proceed to examine three methods of complexity reduction. While none of these methods is as fast as those of Chapter 7, they all have their own particular advantages. The second method, based on the fast Fourier transform, for example, applies to most of the special functions.

10.2.1 Acceleration Based on Functional Equations

The exponential satisfies the functional equation

(10.2.1) $$f(2z) = [f(z)]^2.$$

This allows us to reduce the calculation of the exponential to a small region about the origin and then to approximate in that region using a Taylor or a Padé approximant. From estimates like those of Section 10.1 and (10.2.1) we have

(10.2.2) $$\left|e^z - \left[s_n\left(\frac{z}{2^n}\right)\right]^{2^n}\right| \leq \frac{1}{n!2^{n^2}} \qquad |z| \leq 1$$

and

(10.2.3) $$\left|e^z - \left[r_{n,n}\left(\frac{z}{4^n}\right)\right]^{4^n}\right| \leq \frac{1}{16^{n^2}}\frac{n!n!}{(2n)!(2n)!} \qquad |z| \leq 1$$

where s_n and $r_{n,n}$ are, respectively, the nth Taylor polynomial and the (n, n) Padé approximant to exp at zero. Both of these above estimates provide

$$O_{\text{op}}(\sqrt{n}) \qquad \text{and} \qquad O_B(\sqrt{n}M(n))$$

methods for the evaluation of exp.

The functional relation for log is

(10.2.4) $$f(z^2) = 2f(z)$$

Combined with (10.1.19), this leads to

(10.2.5) $$2^n \log(z^{2^{-n}}) = 2^{n+1}\sum_{k=0}^{\infty}\frac{1}{2k+1}\left(\frac{z^{2^{-n}}-1}{z^{2^{-n}}+1}\right)^{2k+1}.$$

Truncation after n terms leads to an approximation on $|z-1| < \frac{1}{2}$ that has error $O(4^{-n^2})$ and yields an algorithm for log with complexity

$$O_{\text{op}}(\sqrt{n}) \qquad \text{and} \qquad O_B(\sqrt{n}M(n)).$$

These are good intermediate range estimates of exp and log. For

$n := 100$, (10.2.3) provides in excess of 12,000-digit accuracy at the expense of roughly 300 full precision multiplications. (300 terms of the Taylor series provides roughly 600 digits.)

Variations of the above methods can be used to construct $O_{op}(\sqrt{n})$ algorithms for the circular functions and their inverses. (See Exercise 2.) Since any elliptic function (Section 1.7) satisfies an algebraic "half-angle" formula, we can, as above, construct $O_{op}(n^{1/2+\varepsilon})$ algorithms for elliptic functions provided we have expansions available at the origin. (Unfortunately, convenient closed forms of the Taylor series for sn, for example, are not available.)

10.2.2 *Acceleration Based on the FFT*

It is possible, based on FFT methods, to evaluate a polynomial or rational function of degree n at $n+1$ distinct points in $O_{op}(n(\log n)^2)$. (See Exercise 3 of Section 6.2.) Our aim is to use this observation to accelerate the evaluation of partial sums or related approximations. We illustrate with log. Start with

(10.2.6) $$-\log(1-z) = z + \tfrac{1}{2}z^2 + \tfrac{1}{3}z^3 + \cdots$$

and consider

(10.2.7) $$s_{n^2}(z) := \sum_{k=1}^{n^2} \frac{z^k}{k}.$$

We can write

(10.2.8) $$s_{n^2}(z) = \sum_{k=0}^{n-1} z^{kn} p_n(kn)$$

where

(10.2.9) $$p_n(y) = \sum_{j=1}^{n} \frac{z^j}{j+y}.$$

Now, for fixed z, evaluate $p_n(kn)$ at $k = 0, 1, \ldots, n-1$ in $O_{op}(n(\log n)^2)$ (Exercise 4) and evaluate s_{n^2} in a further $O(n)$ operation. Since for $|z| \le \frac{1}{2}$, $s_{n^2}(z)$ provides $\Omega(n^2)$ digits of $\log z$, we have constructed an algorithm for log which is $O_{op}(n^{1/2}(\log n)^2)$.

With care, this idea can be extended to produce

(10.2.10) $$O_{op}(n^{1/2}(\log n)^2) \quad \text{and} \quad O_B(n^{1/2}(\log n)^2 M(n))$$

algorithms for a variety of nonelementary transcendental functions. Almost any function with regular Taylor coefficients is susceptible to such analysis.

Algorithms for the gamma function and the hypergeometric functions, of complexity given by (10.2.10), are presented in Exercises 6 and 7.

We can combine the methods of Section 10.2.1 with the above to construct an

(10.2.11) $$O_{op}(n^{1/3}(\log n)^2) \quad \text{and} \quad O_B(n^{1/3}(\log n)^2 M(n))$$

algorithm for log. This merely requires truncating (10.2.5), say, after n^2 terms and evaluating the truncation using the FFT method in $O_{op}(n(\log n)^2)$ steps. Note that this approximation provides $O(n^3)$ digits of log.

Likewise algorithms can be constructed for exp and the trigonometric functions with complexity given by (10.2.11).

The relative difficulty of implementing these algorithms renders them largely of theoretical interest.

10.2.3 *Acceleration Based on Binary Splitting*

If we wish to evaluate the constant e by summing the Taylor series at 1, then we can and should take advantage of the reduced length of each individual operation. With this in mind consider

(10.2.12) $$p(a,b) := b!/a!$$

and

(10.2.13) $$c(a,b) := p\left(\frac{a+b}{2}, b\right) c\left(a, \frac{a+b}{2}\right) x^{(b-a)/2} + c\left(\frac{a+b}{2}, b\right)$$

where

$$c(a, a+1) := (a+1)x.$$

By construction,

(10.2.14) $$\frac{c(0,2^n)}{(2^n)!\,x^{2^n}} = \sum_{k=0}^{2^n-1} \frac{x^{-k}}{k!}.$$

With $x := 1$, (10.2.14) approximates e with an error of less than $e/(2^n)!$, and hence provides $\Omega(n2^n)$ digits of e. We can use (10.2.13) to recursively evaluate e with bit complexity $O_B((\log n)M(n))$.

Brent [76c] shows how to modify this to provide an $O_B((\log n)^2 M(n))$ algorithm for exp. This is outlined in Exercise 8.

Modifications and variations lead to $O_B((\log n)^2 M(n))$ algorithms for all the elementary functions. Particular values of various of the nonelementary special functions are also amenable to this analysis. So, for example, is

Euler's constant. [See Exercises 10 and 11.] Exercise 9 outlines an $O_B((\log n)^2 M(n))$ algorithm for π based on recursive evaluation of arctan.

It is perhaps worth underlining the observation that these acceleration methods apply only to the bit complexity. The operational complexity is not reduced. Nonetheless, the algorithm for the number e implicit in (10.2.12), (10.2.13), and (10.2.14) is asymptotically as fast as any known and has the virtue of being implementable using only integer addition and multiplication, except for a single final division.

Walz [Pr] has studied classes of asymptotic methods using extrapolation and elimination techniques. These often outperform AGM-based methods in the "microcomputer range" (less than 20 digits). Interestingly, for the complete elliptic integral of the first kind he finds the AGM to be always superior. For incomplete integrals this is not always so.

Comments and Exercises

Much of the material of this section is due to Brent [76*c*]. In particular, Exercises 3 and 8 follow Brent closely.

1. a) Show that truncating the series in (10.1.14) and using Horner's rule leads to an $O_{\text{op}}(n/\log n)$ algorithm for exp.
b) Show that (10.1.18), (10.1.19), and (10.1.20) all lead to $O_{\text{op}}(n)$ algorithms for log using usual methods for evaluating the polynomials or rational functions in question.
c) Show, for $n := 2^n$ and $\delta := 1/2^n$, that (10.1.17) and (10.1.22) lead to $O_{\text{op}}(n)$ algorithms for exp and log.
d) Analyze the complexity of (10.1.15), (10.1.16), and (10.1.21).
Assume in all parts that the method in question is used on a compact region bounded away from the boundary of the domain of convergence.

2. a) Use the functional relation

$$\text{(10.2.15)} \qquad 2\arctan\left(\frac{z}{\sqrt{z^2+1}+1}\right) = \arctan z$$

and the expansion

$$\arctan z = \sum_{k=0}^{\infty} \frac{(-1)^k z^{2k+1}}{2k+1} \qquad |z|<1$$

to construct on $O_{\text{op}}(n^{1/2})$ algorithm for arctan on $|z| \le \eta \le 1$.
b) Use the functional relation

$$\text{(10.2.16)} \qquad \left[\cos\left(\frac{z}{2}\right)\right]^2 = \frac{\cos z + 1}{2}$$

to construct an $O_{\text{op}}(n^{1/2})$ algorithm for cos on D_1:

c) Show, in general, that if

$$f(z) = \sum_{n=0}^{\infty} a_n z^n \qquad |z| < 1 + \delta$$

and $f(z/2)$ is an algebraic function of $f(z)$, then one can construct an algorithm of complexity

$$O_{\text{op}}(n^{1/2}) \qquad \text{and} \qquad O_B(n^{1/2}M(n))$$

on D_1.

3. Instead of approximating $e^{z/2^n}$ by $s_n(z/2^n)$ in (10.2.2), approximate $e^{z/2^n} - 1$ by $s_n(z/2^n) - 1$. Then repeatedly use the relation

$$(1+\varepsilon)^2 - 1 = 2\varepsilon + \varepsilon^2$$

to evaluate $e^z - 1$. Show that this avoids requiring $O(n^{1/2})$ guard digits.

This modification and its obvious analogue for the Padé approximant allow the calculation of exp without loss of significant digits beyond the $O(\log n)$ loss inherent in performing $n^{1/2}$ operations.

4. Show that $p_n(y)$ of (10.2.9) can be written as

$$p_n(y) = \frac{w_n(y)}{v_n(y)}$$

where w_n and v_n are polynomials of degree n. Use FFT methods to show that the coefficients of w_n and v_n can all be calculated in $O_{\text{op}}(n(\log n)^2)$ and hence, that $p_n(y)$ can be evaluated at n points in $O_{\text{op}}(n(\log n)^2)$. (See Exercise 1b) of Section 6.2.)

5. a) Construct an $O_{\text{op}}(n^{1/2}(\log n)^2)$ algorithm for exp by writing

$$\sum_{n=0}^{N^2-1} \frac{x^n}{n!} = t_N(0) + \cdots + t_N(N-1)$$

where

$$t_N(m) := \frac{x^{Nm}}{(Nm)!}\left[1 + \frac{x}{Nm+1} + \frac{x^2}{(Nm+1)(Nm+2)} + \cdots + \frac{x^{N-1}}{(Nm+1)\cdots(N(m+1)-1)}\right]$$

and evaluating $t_N(m)$ for $m = 0, \ldots, N-1$. Care must be taken to compute $(Nk)!$ in the requisite time.
b) Show how part a) can be used to construct an $O_{\text{op}}(n^{1/3}(\log n)^2)$ algorithm for exp.

c) Construct an $O_{op}(n^{1/2}(\log n)^2)$ algorithm for the *Bessel function of order zero*,

$$J_0(z) := \sum_{k=0}^{\infty} \frac{(-1)^k z^{2k}}{2^{2k} k! k!}. \tag{10.2.17}$$

6. (*An* $O_{op}(n^{1/2}(\log n)^2)$ *algorithm for the gamma function*)

a) From the definition

$$\Gamma(s) := \int_0^\infty e^{-t} t^{s-1}\, dt$$

show, by breaking the integral at N and expanding, that

$$\Gamma(s) = N^s \sum_{k=0}^{\infty} \frac{(-1)^k}{k!} \frac{N^k}{s+k} + \int_N^\infty e^{-t} t^{s-1}\, dt. \tag{10.2.18}$$

b) Show for $s \in [1, 2]$ that

$$\left|\Gamma(s) - N^s \sum_{k=0}^{6N} \frac{(-1)^k}{k!} \frac{N^k}{s+k}\right| \le 2Ne^{-N}.$$

c) Use b) and FFT methods to construct an algorithm for the gamma function of complexity

$$O_{op}(n^{1/2}(\log n)^2) \quad \text{and} \quad O_B(n^{1/2}(\log n)^2 M(n)).$$

7. ($O_{op}(n^{1/2}(\log n)^2)$ *algorithms for hypergeometric functions*) We now consider a (*general*) *hypergeometric function* to be a function

$$f(z) := 1 + \sum_{n=1}^{\infty} a_n z^n \tag{10.2.19}$$

where $a_n/a_{n-1} := R(n)$ for some fixed rational function R. In this problem R is assumed to have rational (or precomputed) coefficients and f is assumed to have a nonzero radius of convergence.

a) Show that the Gaussian hypergeometric series $F(a, b; c; z)$ of (1.3.5) is hypergeometric by the above definition. Show that, provided a, b, and c, $c \neq 0, -1, -2, \ldots$, are rational, $F(a, b; c; z)$ satisfies the additional assumptions.

b) Show that $\sin(\sqrt{z})$, e^z, $\log(1-z)$, E/π, and K/π are all hypergeometric functions, up to a rational normalization.

c) For fixed n let

$$S_{n^2-1}(z) := \sum_{k=0}^{n^2-1} a_k z^k$$

$$T(k) := \prod_{i=0}^{k-1} R(i) \qquad R(0) := 1$$

and

$$Q(k) := R(k) + R(k)R(k+1)z + \cdots + R(k)R(k+1)\cdots R(k+n-1)z^{n-1}.$$

Observe that

$$a_k = \prod_{i=0}^{k} R(k)$$

and show that

$$S_{n^2-1} = Q(0) + z^n Q(n)T(n) + z^{2n}Q(2n)T(2n) + \cdots + z^{n(n-1)}Q(n(n-1))T(n(n-1)).$$

d) Show that

$$T(n), T(2n), \ldots, T(n(n-1))$$

can all be evaluated in $O_{op}(n(\log n)^2)$.
Hint: Consider the rational function of y

$$V(y) := \prod_{i=0}^{n-1} R(i+y)$$

and observe that

$$T(kn) = V(0)\cdot V(n) \cdots V((k-1)n).$$

Now first compute the coefficients of V by recursively breaking the problem in half and using a fast multiplication. Then calculate V at the points $V(0)$, $V(n)$, $V(2n), \ldots, V((n-1)n)$. (See Exercises 1 and 3 of Section 6.2.)

e) Show that

$$Q(0), Q(n), \ldots, Q((n-1)n)$$

can all be evaluated in $O_{op}(n(\log n)^2)$.

Hint: Note that Q is a rational function of k of degree bounded by $n \cdot \text{degree}(R)$. Now show that the coefficients of Q as functions of k can be calculated in $O_{\text{op}}(n(\log n)^2)$ by proceeding recursively. To do this consider

$$\begin{aligned} &R(k) + [R(k)R(k+1)]z + \cdots \\ &\quad + [R(k)R(k+1)\cdots R(k+2n-1)]z^{2n-1} \\ &= \{R(k) + \cdots + [R(k)R(k+1)\cdots R(k+n-1)]z^{n-1}\} \\ &\quad + \left[z^n \prod_{i=k}^{k+n-1} R(i)\right]\{R(k+n) + \cdots + [R(k+n) \\ &\quad \times R(k+n+1)\cdots R(k+2n-1)]z^{n-1}\} \end{aligned}$$

and use a fast polynomial multiplication to recombine the pieces. Finally evaluate $Q(0), Q(n), \ldots, Q((n-1)n)$ as before.

f) Use the preceding parts to construct

$$O_{\text{op}}(n^{1/2}(\log n)^2) \quad \text{and} \quad O_B(n^{1/2}(\log n)^2 M(n))$$

algorithms for any hypergeometric function.

8. *(An $O_B(\log n)^2 M(n))$ algorithm for exp)*

a) Show that (10.2.13) can be used to recursively evaluate e with bit complexity $O_B((\log n)M(n))$.

b) Use (10.2.13) for rational p/q, where $p^2 \le q \le 2^N$, to compute $e^{p/q}$. Show that the bit complexity is as in Exercise 8a).

c) Suppose $x \in [0, 1)$ is a binary 2^m-digit number. Show that x can be written as

$$x = \sum_{k=0}^{m} \frac{p_k}{q_k}$$

where $q_k := 2^{2^k}$ and $0 \le p_k < 2^{2^{k-1}}$.

d) Write

$$e^x = \prod_{k=0}^{m} e^{p_k/q_k}$$

with p_k and q_k as in c). Show that this gives an $O_B((\log n)^2 M(n))$ algorithm for exp on $[0, 1)$.

9. *(An $O_B(\log n)^2 M(n))$ algorithm for π)*

a) Consider the expansion

$$\arctan\left(\frac{1}{x}\right) = \frac{(1/x)^1}{1} - \frac{(1/x)^3}{3} + \frac{(1/x)^5}{5} - \cdots$$

and the recursion

$$\begin{aligned} c(a, a+1) &:= -x^2 \\ c(a, b) &:= p\left(\frac{a+b}{2}, b\right)c\left(a, \frac{a+b}{2}\right)(-x^2)^{(b-a)/2} \\ &\quad + p\left(a, \frac{a+b}{2}\right)c\left(\frac{a+b}{2}, b\right) \end{aligned}$$

where, for $a < b$,

$$p(a, b) := (2a+1)\cdot(2a+3)\cdots(2b-1)\,.$$

Show that

$$\frac{c(0, 2^n)}{x^{2^{n+1}+1}p(1, 2^n)}$$

calculates the $(2^{n+1}-1)$th partial sum of $\arctan(1/x)$.

b) Show that for a fixed integer $x > 1$ the above recursion computes $\arctan(1/x)$ in

$$O_B((\log n)^2 M(n))\,.$$

This gives an $O_B((\log n)^2 M(n))$ algorithm for π from

$$\pi = 16\arctan\left(\tfrac{1}{5}\right) - 4\arctan\left(\tfrac{1}{239}\right)$$

or any similar arctan formula.

10. a) Let f be a hypergeometric function defined as in Exercise 7 (with the same additional assumptions). Show, for fixed p/q rational inside the region of convergence of the expansion (10.2.19), that $f(p/q)$ can be calculated with bit complexity

$$O_B((\log n)^2 M(n))\,.$$

b) Show, for fixed rational p/q, that $\Gamma(p/q)$ can be calculated with bit complexity

$$O_B((\log n)^2 M(n))\,.$$

11. (*On the complexity of Euler's constant*) *Euler's constant* or the *Euler–Mascheroni constant* γ is defined by

$$\gamma := \lim_{m\to\infty}\left[1+\frac{1}{2}+\frac{1}{3}+\cdots+\frac{1}{m}-\log m\right]=0.5772156649\ldots$$

(10.2.20)

It is related to the gamma function by the formula

$$\frac{1}{\Gamma(z)} = ze^{\gamma z}\left[\prod_{n=1}^{\infty}\left(1+\frac{z}{n}\right)e^{-z/n}\right]. \tag{10.2.21}$$

a) Use the recursion

$$\Gamma(z+1)=z\Gamma(z)$$

to prove that if Γ has an expansion of form (10.2.21), then γ is given by (10.2.20).

b) The *exponential integral* E_1 is defined by

$$E_1(x)=\int_x^{\infty}\frac{e^{-t}\,dt}{t}. \tag{10.2.22}$$

Show that

$$-E_1(x)=\gamma+\log x+\sum_{k=1}^{\infty}\frac{(-x)^k}{k\cdot k!}\qquad x>0. \tag{10.2.23}$$

c) Use (10.2.23) to construct an

$$O_B((\log n)^2M(n))$$

algorithm for γ by choosing x roughly of size $6n$.

This method, suggested by Sweeney [63], is a reasonably efficient method for computing γ. Brent and McMillan [80] present a number of algorithms for this computation. They calculate over 29,000 partial quotients of the continued fraction for γ. As a consequence they show that if γ is rational the denominator of γ exceeds $10^{15,000}$.

Chapter Eleven

Pi

Abstract. *The first section of the chapter deals with the history of the calculation of π and related matters, while the second section deals with its transcendence. The third section looks at irrationality measures and includes a proof of the irrationality of $\zeta(3)$. This chapter is largely self-contained and indeed contains considerable related number theory, especially in the exercises.*

11.1 *ON THE HISTORY OF THE CALCULATION OF* π

The history of π presumably begins with man's first attempts at estimating the perimeter or area of a circle of given radius and as such starts at the dawn of recorded history. The Egyptian Rhind (or Ahmes) Papyrus which dates from approximately 2000 B.C., gives a value of $(16/9)^2 = 3.1604\ldots$ for π. Various other early Babylonian and Egyptian estimates include 3, $3\frac{1}{8}$, and $3\frac{1}{7}$. Implicit in the Bible (1 Kings 7: 23) is a value 3: "And he made a molten sea, ten cubits from the one brim to the other; it was round all about... and a line of thirty cubits did compass it round about."

Mathematical interest in π comes into sharp focus in the classical Greek period. The Greeks investigated the problem of "squaring the circle." This question and its final resolution over two millenia later will be pursued in the next section. Currently we wish to review the primary Western developments in the calculation of π.

Archimedes of Syracuse (287–212 B.C.) provided the first major landmark in the quest for digits of π. By considering inscribed and circumscribed polygons of 96 sides, Archimedes gave the estimate

$$3\frac{10}{71}<\pi<3\frac{1}{7}.$$

A salient feature of Archimedes' method is that it can, in principle, be used to provide any number of digits of π.

If a_n denotes the length of a circumscribed regular $6 \cdot 2^n$-gon and b_n denotes the length of an inscribed regular $6 \cdot 2^n$-gon about a circle of radius 1/2, then

$$(11.1.1) \qquad a_{n+1} = \frac{2a_n b_n}{a_n + b_n}$$

$$(11.1.2) \qquad b_{n+1} = \sqrt{a_{n+1} b_n}\,.$$

This two-term iteration, starting with $a_0 := 2\sqrt{3}$ and $b_0 := 3$, can be used to calculate π. (See also Section 8.4.) The fourth iteration yields $a_4 = 3.1427\ldots$ and $b_4 = 3.1410\ldots$ and corresponds to estimating π using polygons with 96 sides.

If we observe that

$$(11.1.3) \qquad a_{n+1} - b_{n+1} = \frac{a_{n+1} b_n}{(a_{n+1} + b_{n+1})(a_n + b_n)} (a_n - b_n)$$

we again see that the error is decreased by a factor of approximately 4 with each iteration. Variations of this modern formulation of Archimedes' method provided the basis for virtually all extended precision calculations of π for the next 1800 years, culminating with Ludolph van Ceulen (1540–1610) who correctly computed 34 digits. The limitations of this method stem from the relatively slow convergence and from the need to extract square roots. (See Exercise 1.)

François Vièta (1540–1603) gave the first infinite expansion

$$(11.1.4) \qquad \frac{2}{\pi} = \sqrt{\frac{1}{2}} \sqrt{\frac{1}{2} + \frac{1}{2}\sqrt{\frac{1}{2}}} \sqrt{\frac{1}{2} + \frac{1}{2}\sqrt{\frac{1}{2} + \frac{1}{2}\sqrt{\frac{1}{2}}}} \cdots$$

which he derived by considering a limit of areas of inscribed 2^n-gons. (See Exercise 2.) John Wallis (1616–1703) through a complicated calculation demanding prodigious numerical insight derived the infinite product expansion

$$(11.1.5) \qquad \frac{\pi}{2} = \frac{2 \cdot 2 \cdot 4 \cdot 4 \cdot 6 \cdot 6 \cdot 8 \cdot 8 \cdots}{1 \cdot 3 \cdot 3 \cdot 5 \cdot 5 \cdot 7 \cdot 7 \cdot 9 \cdots}\,.$$

This appears in his *Arithmetica Infinitorum* of 1655. A few years later Lord Brouncker (1620–1684), the first president of the Royal Society, recast this as the continued fraction.

$$(11.1.6) \qquad \pi = \cfrac{4}{1 + \cfrac{1}{2 + \cfrac{9}{2 + \cfrac{}{2 + \cfrac{49}{2 + \cdots}}}}}\,.$$

25 missing

The Scottish mathematician James Gregory (1638–1675) in 1671 provided the underlying method for the next era in the history of the calculation of π. He showed that

$$(11.1.7) \qquad \arctan x = \int_0^x \frac{dx}{1 + x^2} = x - \frac{x^3}{3} + \frac{x^5}{5} - \frac{x^7}{7} + \cdots$$

and hence, on setting $x := 1$, that

$$(11.1.8) \qquad \frac{\pi}{4} = 1 - \frac{1}{3} + \frac{1}{5} - \frac{1}{7} + \cdots$$

a formula independently discovered in 1674 by Leibniz (1646–1716). By the beginning of the eighteenth century Abraham Sharp under the direction of the English astronomer and mathematician E. Halley had obtained 71 correct digits of π using Gregory's series (11.1.7) with $x := \sqrt{1/3}$, namely,

$$(11.1.9) \qquad \frac{\pi}{6} = \frac{1}{\sqrt{3}} \left(1 - \frac{1}{3 \cdot 3} + \frac{1}{3^2 \cdot 5} - \frac{1}{3^3 \cdot 7} + \cdots\right).$$

It is the techniques of calculus that so expanded the scope for calculating, and it is perhaps not surprising that Isaac Newton (1642–1727) himself calculated π to 15 digits sometime in 1665–66. He used the series

$$(11.1.10) \qquad \pi = \frac{3\sqrt{3}}{4} + 24\left(\frac{1}{12} - \frac{1}{5 \cdot 2^5} - \frac{1}{28 \cdot 2^7} - \frac{1}{72 \cdot 2^9} - \cdots\right)$$

which is essentially an arcsin expansion. (See Exercise 4.) Newton was later to write: "I am ashamed to tell you to how many figures I carried these computations, having no other business at the time." John Machin (1680–1752) derived the formula which bears his name:

$$(11.1.11) \qquad \frac{\pi}{4} = 4 \arctan\left(\frac{1}{5}\right) - \arctan\left(\frac{1}{239}\right).$$

Coupled with Gregory's series for arctan this provides a very attractive method for calculating π since the first term is well suited to decimal arithmetic and the second term converges very rapidly. Machin calculated 100 digits this way in 1706. In the same year William Jones published his *A*

New Introduction to the Mathematics, where he denoted the ratio of the circumference to the diameter by the Greek letter π, presumably for the first letter of periphery. It was, however, Leonard Euler (1707–1783) who popularized the use of the symbol. Euler derived numerous series and products for π and π^2. Among the best-known are

$$\text{(11.1.12)} \qquad \frac{\pi^2}{6} = \sum_{n=1}^{\infty} \frac{1}{n^2}$$

and

$$\text{(11.1.13)} \qquad \frac{\pi^4}{90} = \sum_{n=1}^{\infty} \frac{1}{n^4}.$$

The explicit summation of (11.1.12) had eluded Liebniz and also the Bernoulli brothers, Jacques and Jean. The method by which Euler derived his evaluations of $\Sigma_{n=1}^{\infty} 1/n^{2k}$ is outlined in Exercise 7. This is to be found in Euler's *Introducio in Analysin Infinitorum* of 1748. The Machin-like formula

$$\text{(11.1.14)} \qquad \pi = 20 \arctan\left(\frac{1}{7}\right) + 8 \arctan\left(\frac{3}{79}\right)$$

coupled with the expansion

$$\text{(11.1.15)} \qquad \arctan x = \frac{y}{x}\left(1 + \frac{2}{3}y + \frac{2\cdot 4}{3\cdot 5}y^2 + \cdots\right)$$

where $y := x^2/(1+x^2)$, allowed Euler to compute 20 digits of π in under an hour.

The next 200 years saw little change in the methods employed to calculate π. In 1844 Johann Dase (1824–1861), a calculating prodogy, used the formula

$$\text{(11.1.16)} \qquad \frac{\pi}{4} = \arctan\left(\frac{1}{2}\right) + \arctan\left(\frac{1}{5}\right) + \arctan\left(\frac{1}{8}\right)$$

to produce 205 digits of π. (Dase's arithmetical abilities were awesome—he could multiply 100-digit numbers together in his head, a feat which took him roughly 8 hours.)

The zenith (or nadir depending on your perspective) in premachine calculations was achieved by William Shanks (1812–1882), who published 607 purported digits of π, of which 527 were correct. Later Shanks published an extension to 707 digits. This was also incorrect after the 527th digit. These calculations took Shanks years and were performed in an entirely straightforward fashion using no tricks or shortcuts. (See W. Shanks [1853].) The mistakes went unnoticed until 1945, when D. F. Ferguson, in one of the final hand calculations, produced 530 digits. Ferguson produced 808 digits in 1947, using a desk calculator and the formula

$$\text{(11.1.17)} \qquad \frac{\pi}{4} = 3 \arctan\left(\frac{1}{4}\right) + \arctan\left(\frac{1}{20}\right) + \arctan\left(\frac{1}{1985}\right).$$

Thus dawns the computer age. In June 1949 ENIAC (Electronic Numerical Integrator and Computer) was used to evaluate 2037 digits of π using Machin's formula and 70 hours elapsed time. An analysis of the distribution of the digits was carried out by Metropolis, Reitwiesner, and von Neumann. By 1958, Genuys had computed 10,000 digits on an IBM 704 in 100 minutes, once again using Machin's formula. Felton had performed a 10,000-digit calculation in 1957; however, due to machine error it was only correct to 7480 digits. In 1961 D. Shanks and Wrench [62] used the identity

$$\text{(11.1.18)} \qquad \pi = 24 \arctan\left(\frac{1}{8}\right) + 8 \arctan\left(\frac{1}{57}\right) + 4 \arctan\left(\frac{1}{239}\right)$$

and under 9 hours on an IBM 7090 to produce 100,000 digits of π. This was checked using the formula

$$\text{(11.1.19)} \qquad \pi = 48 \arctan\left(\frac{1}{18}\right) + 32 \arctan\left(\frac{1}{57}\right) - 20 \arctan\left(\frac{1}{239}\right).$$

The million-digit mark was set by Guilloud and Bouyer in 1973 on a CDC 7600. The calculation, which took just under a day, used (11.1.19) with (11.1.18) as a check.

Kanada, Tamura, Yoshino, and Ushiro [Pr] calculated in excess of 16 million digits using an AGM based algorithm, Algorithm 2.2, and checked 10 million digits using (11.1.19). The 16 million-digit calculation took under 30 hours on a HITAC M-280H and used an FFT-based fast multiplication.

At the end of 1985 the record belonged to W. Gosper. He calculated 17 million terms of the continued fraction expansion for π and so in excess of this number of decimal digits—after a radix conversion from a binary computation. His method is based on a very careful evaluation of Ramanujan's series (5.5.23) on a Symbolics 3670. (A remarkable feat considering the size of the machine.) As is surprisingly often the case with these large scale calculations, Gosper uncovered subtle design flaws which had not surfaced in smaller calculations.

In January 1986, D. H. Bailey [Pr] computed 29,360,000 decimal digits of π on the CRAY-2 at the NASA Ames Research Center. This calculation used only 12 steps of the quartic algorithm (5.4.7) with $r := 4$. This results in computing $\alpha(2^{50})$, which agrees with π^{-1} to more than 45 million places. The calculation took less than 28 hours and was verified with a 40-hour computation of 25 steps of Algorithm 2.1. It is amusing to observe that the quartic calculation requires well under 100 full precision multiplications, divisions, and root extractions.

In July 1986, Kanada reclaimed the record with a computation of 2^{25} decimal digits. He again used Algorithm 2.2, verified in September using (5.4.7) with $r := 4$, but reduced the elapsed time to 5 hours and 56 minutes on a S-810/20 super computer. This represented a speed-up by a factor of

15. His previous computation now used only 96 minutes of CPU time. Plans were to compute 2^{27} decimal digits (over 100 million) at the end of 1987.

Nor is the end in sight. It will probably be the case than hundreds or thousands of millions of digits will be calculated by the end of the century. (This is now more a matter of will than anything else.) Apart from observations like "the sequence 314159 appears in the digits of π commencing at digit 9,973,760," there is little we care to say about the digits. They have, however, been subjected to considerable scrutiny. It is an open question as to whether π is *normal*. That is, do all sequences of integers appear with the same frequency in the digits (are one-tenth of the digits 7, one-hundredth of the consecutive digit pairs 23, etc.)? On the basis of the first 30 million digits the answer appears positive. This, of course, is no great help in deciding the normality issue. (See Wagon [85].)

In terms of utility, even far-fetched applications such as measuring the circumference of the universe require no more digits than Ludolph van Ceulen had available—but then utility has had little to do with this particular story.

Comments and Exercises

This section presents only the highlights of the quest for digits. The matter may be pursued in detail in Beckmann [77], a most useful though rather individualistic history, and in *Le Petit Archimède* [80]. Schepler's chronography [50] and Wrench's history [60] are also of interest. Details of the more recent calculations may be found in Tamura and Kanada [Pr], where a compendium of Machin-like identities is provided.

There is also a considerable collection of π-related trivia. For example, the Indiana House of Representatives attempted to legislate the value of π in Bill 246 of 1897. The bill, which appears to proclaim π to be several different incredibly inaccurate values, including 4 and 64/25 (see Beckmann [77], and Singmaster [85]), passed the House and only floundered in the Senate on the apparently chance intercession of C. A. Waldo, a professor at Purdue. Keith [86] gives a 402 digit mnemonic for π.

1. a) Show that the algorithm of (11.1.1) and (11.1.2) calculates π by showing that a_n and b_n are as advertised.

b) Prove (11.1.3) and estimate how many iterations of (11.1.1) and (11.1.2) are required to calculate 35 digits of π. This should be compared to Bailey's [Pr] calculation which uses the same operations.

2. a) Prove, from the product expansions for sin and cos, that

$$\theta = \frac{\sin\theta}{\cos(\theta/2)\cos(\theta/2^2)\cos(\theta/2^3)\cdots} \qquad |\theta| < \pi. \tag{11.1.20}$$

b) Alternatively deduce (11.1.20) in an elementary fashion by setting

$$I_n := \cos\left(\frac{\theta}{2}\right)\cos\left(\frac{\theta}{2^2}\right)\cdots\cos\left(\frac{\theta}{2^n}\right)$$

and showing that

$$I_n = \frac{\sin\theta}{2^n\sin(\theta/2^n)}.$$

c) Set $\theta := \pi/2$ and use the formula $\cos(\theta/2) = \sqrt{\frac{1}{2} + \frac{1}{2}\cos\theta}$ to deduce Vièta's formula (11.1.4)

$$\frac{2}{\pi} = \sqrt{\frac{1}{2}}\sqrt{\frac{1}{2} + \frac{1}{2}\sqrt{\frac{1}{2}}}\sqrt{\frac{1}{2} + \frac{1}{2}\sqrt{\frac{1}{2} + \frac{1}{2}\sqrt{\frac{1}{2}}}}\cdots.$$

3. a) Prove Wallis's formula (11.1.5) in the form

$$\frac{\pi}{2} = \frac{2\cdot2\cdot4\cdot4\cdot6\cdot6\cdot8\cdot8}{1\cdot3\cdot3\cdot5\cdot5\cdot7\cdot7\cdot9}\cdots.$$

Hint: Show that

$$\int_0^{\pi/2}\sin^{2m}x\,dx = \frac{1\cdot3\cdot5\cdots(2m-1)}{2\cdot4\cdot6\cdots2m}\,\frac{\pi}{2}$$

and

$$\int_0^{\pi/2}\sin^{2m+1}x\,dx = \frac{2\cdot4\cdot6\cdots2m}{1\cdot3\cdot5\cdots(2m+1)}.$$

b) Establish the corresponding formula for e:

$$\frac{e}{2} = \left(\frac{2}{1}\right)^{1/2}\left(\frac{2\cdot4}{3\cdot3}\right)^{1/4}\left(\frac{4\cdot6\cdot6\cdot8}{5\cdot5\cdot7\cdot7}\right)^{1/8}\cdots.$$

c) Show that the volume of the $2n$-dimensional unit sphere is $\pi^n/n!$ while the $(2n+1)$-dimensional unit sphere has the volume $2^{2n+1}[n!/(2n+1)!]\pi^n$. Find a unified formula for these two cases.

4. Deduce (11.1.10) roughly as Newton did. Show that

$$\frac{\pi}{24} - \frac{\sqrt{3}}{32} = \int_0^{1/4}\sqrt{x - x^2}\,dx$$

and that

$$\int_0^{1/4}\sqrt{x-x^2}\,dx = \int_0^{1/4}\sqrt{x}(\sqrt{1-x})\,dx$$
$$= \frac{2}{3\cdot2^3} - \frac{1}{5\cdot2^5} - \frac{1}{28\cdot2^7} - \cdots.$$

5. a) Deduce Machin's formula

$$\frac{\pi}{4} = 4 \arctan\left(\frac{1}{5}\right) - \arctan\left(\frac{1}{239}\right)$$

as follows. Let $\theta := \arctan \frac{1}{5}$. Then

$$\tan 2\theta = \frac{2 \tan \theta}{1 - \tan^2 \theta} = \frac{5}{12}$$

and

$$\tan 4\theta = \frac{120}{119} = 1 + \frac{1}{119}.$$

Hence

$$\tan\left(4\theta - \frac{\pi}{4}\right) = \frac{-1 + \tan 4\theta}{1 + \tan 4\theta} = \frac{1}{239}.$$

b) Show that arctan satisfies the addition formula

$$\arctan x + \arctan y = \arctan\left(\frac{x+y}{1-xy}\right) \qquad xy < 1.$$

c) Show that

$$\text{(11.1.21)} \quad \arctan\left(\frac{1}{p}\right) = \arctan\left(\frac{1}{p+q}\right) + \arctan\left(\frac{q}{p^2 + pq + 1}\right)$$

and that if $1 + p^2 = qr$,

$$\text{(11.1.22)} \quad \arctan\left(\frac{1}{p+r}\right) + \arctan\left(\frac{1}{p+q}\right) = \arctan\left(\frac{1}{p}\right).$$

Formula (11.1.21) was known to Euler. Bromwich [26] attributes (11.1.22) to Charles Dodgson (Lewis Carroll).

6. (*Machin-like formulae*)

a) Show, for integral a_j and b_j, that

$$k\pi = \arctan\left(\frac{b_1}{a_1}\right) + \arctan\left(\frac{b_2}{a_2}\right) + \cdots + \arctan\left(\frac{b_n}{a_n}\right)$$

where k is an integer if and only if

$$(a_1 + ib_1)(a_2 + ib_2) \cdots (a_n + ib_n)$$

has zero imaginary part.

Hint: Consider $(a_1 + ib_1) \cdots (a_n + ib_n) = re^{i\theta}$, $|\theta| < \pi$, and use the fact that

$$\arctan z = \frac{1}{2i} \log\left(\frac{1+iz}{1-iz}\right).$$

(This gives an algorithmic check for Machin-like formulae.)

b) Show, for positive integral u, v, and k and integral m and n, that

$$m \arctan\left(\frac{1}{u}\right) + n \arctan\left(\frac{1}{v}\right) = \frac{k\pi}{4}$$

if and only if $(1-i)^k (u+i)^m (v+i)^n$ is real.

c) Verify

$$\frac{\pi}{4} = 4 \arctan\left(\frac{1}{5}\right) - \arctan\left(\frac{1}{239}\right) \qquad \text{(Machin, 1706)}$$

$$\frac{\pi}{4} = \arctan\left(\frac{1}{2}\right) + \arctan\left(\frac{1}{3}\right) \qquad \text{(Euler, 1738)}$$

$$\frac{\pi}{4} = 2 \arctan\left(\frac{1}{2}\right) - \arctan\left(\frac{1}{7}\right) \qquad \text{(Hermann, 1706)}$$

$$\frac{\pi}{4} = 2 \arctan\left(\frac{1}{3}\right) + \arctan\left(\frac{1}{7}\right) \qquad \text{(Hutton, 1776)}.$$

These are, in fact, all the nontrivial solutions of b). This was a problem of Gravé's solved by Størmer in 1897. The problem can be reduced to finding integral solutions of $1 + x^2 = 2y^n$ or $1 + x^2 = y^n$, $n \geq 3$, n odd. (See Ribenboim [84].) Much related material on Machin-like formulae occurs in Lehmer [38] and Todd [49].

7. Prove Brouncker's continued fraction by showing that

$$\frac{4}{\pi} = 1 + \cfrac{1}{2 + \cfrac{9}{2 + \cfrac{25}{2 + \cdots}}}.$$

Hint: If

$$s := a_0 + a_1 + a_1 a_2 + a_1 a_2 a_3 + \cdots$$

then

$$s = a_0 + \cfrac{a_1}{1 - \cfrac{a_2}{1 + a_2 - \cfrac{a_3}{1 + a_3 - \cdots}}}.$$

This is a nonsimple continued fraction. The convergents satisfy a similar recursion to that given in Exercise 2 of Section 11.3.

Apply this to

$$\arctan x = x - \frac{x^3}{3} + \frac{x^5}{5} - \frac{x^7}{7} + \cdots$$

so that

$$a_0 = 0, a_1 = x, a_2 = \frac{-x^2}{3}, a_3 = \frac{-3x^2}{5}, \ldots$$

and

$$\arctan x = \cfrac{x}{1 + \cfrac{x^2}{3 - x^2 + \cfrac{9x^2}{5 - 3x^2 + \cfrac{25x^2}{7 - 5x^2 \cdots}}}}.$$

Now set $x := 1$. (According to Beckmann, Brouncker merely announced his result—the above derivation is essentially due to Euler.)

8. Consider the series

$$\sin x = x - \frac{x^3}{3!} + \frac{x^5}{5!} - \cdots. \tag{11.1.23}$$

Observe that $\sin x = 0$ exactly when $x = \pm k\pi$. Now observe that on setting $y := x^2$,

$$1 - \frac{y}{3!} + \frac{y^2}{5!} - \frac{y^3}{7!} + \cdots = 0 \tag{11.1.24}$$

exactly when $y = (k\pi)^2$, $k = 1, 2, 3, \ldots$. If (11.1.24) were a polynomial, we would know that the sum of the reciprocals of the roots of (11.1.23) equals the negative of the coefficient of y and in general the sum of the reciprocals of the powers would be expressible in terms of the coefficients and Bernoulli numbers. Thus we would deduce that

$$\sum_{k=1}^{\infty} \frac{1}{(k\pi)^2} = \frac{1}{6} \quad \text{and} \quad \sum_{k=1}^{\infty} \frac{1}{(k\pi)^4} = \frac{1}{90}.$$

Use the product expansion for sin [Section 2.2, Exercise 1d)] to make the above argument of Euler's rigorous. (See also Exercise 14 of Section 11.3.)

9. In computing π from (11.1.19) one must evaluate $\arctan(\frac{1}{18})$ and $\arctan(\frac{1}{57})$. Use (11.1.15) to observe that

$$\arctan\left(\frac{1}{18}\right) = 18\left(\frac{1}{325} + \frac{2}{3 \cdot 325^2} + \frac{2 \cdot 4}{3 \cdot 5(325)^3} + \cdots\right)$$

and

$$\arctan\left(\frac{1}{57}\right) = 57\left(\frac{1}{3250} + \frac{2}{3(3250)^2} + \frac{2 \cdot 4}{3 \cdot 5(3250)^3} + \cdots\right).$$

Thus terms of the second series are just decimal shifts of terms of the first series. (See Ballantine [39].) How does this affect the complexity of calculating the two arctans?

10. Prove that the number

$$0.12345678910111213 \cdots n(n+1) \cdots$$

is normal. A proof may be found in Niven [56].

11.2 *ON THE TRANSCENDENCE OF* π

The problem of "squaring the circle" is the problem of constructing a square of the same area as a given circle of radius 1, or alternatively given a line segment of unit length of constructing a segment of length $\sqrt{\pi}$. The rules of construction allow for the use of an unmarked straightedge and an unmarked compass. A more precise definition of constructible is provided in Exercise 1. In fact, the constructible numbers are exactly those numbers which can be obtained from the integers by a finite sequence of rational operations and extraction of square roots. (See Exercise 1.) Thus constructible numbers are algebraic and the transcendentality of π shows the impossibility of the problem.

The Greek notion of number, based on geometric construction, made consideration of such problems more natural than they perhaps seem today. Indeed the problem had arisen by the fifth century B.C. Anaxagoras, who died in 428 B.C., had, according to Plutarch, considered it while in jail. His contemporary, Hippocrates of Chios, the author of one of the first geometry texts, also considered the question. The other classical Greek problems of "duplicating the cube" and "trisecting the angle" also arose in this period. The "Delian problem" of duplicating the cube (in volume), so named because the oracle of Apollo at Delos had prescribed duplicating the cubical altar as a means of halting the plague of 428 B.C., is equivalent to constructing $\sqrt[3]{2}$. (The impossibility of solving these problems is also discussed in Exercise 1.)

By 414 B.C. attempts at constructing π had become so numerous that Aristrophanes refers to "circle squarers" in his play "The Birds." The term came to refer to people who attempt the impossible. However, attempting the futile is not always a waste of time. As Boyer [68, p. 71] points out:

The better part of Greek mathematics, and of much later mathematical thought, was suggested by efforts to achieve the impossible—or, failing this, to modify the rules. The Heroic Age failed in its immediate objective, under the rules, but the efforts were crowned with brilliant success in other respects.

It is hard to know whether more energy has been consumed by attempts at circle squaring or by calculations of π. While doomed attempts to square the circle flourish to this day, by the eighteenth century it had become accepted in the mathematical community that the problem was probably impossible. In 1755 the French Academy of Sciences refused to examine any more quadratures while as early as 1668 Gregory had attempted to prove their impossibility. The first substantial step in this direction was due to Lambert (1728–1777), who proved π irrational in 1761. A subsequent more rigorous proof was provided by Legendre (1752–1833). Legendre proved the irrationality of π^2 in his *Eléments de Géométrie* of 1794 and commented:

> It is probable that the number π is not even contained among the algebraic irrationalities . . . But it seems to be very difficult to prove this strictly.

(See Exercise 3.) This belief was shared by Euler. Liouville established the existence of transcendental numbers in 1840, and in 1873 Hermite proved e transcendental. It had been proved irrational by Euler in 1737. Finally in 1882 F. Lindemann [1882] extended Hermite's proof to cover the transcendence of π, thus laying to rest a 2300-year-old problem. This was simplified by Weierstrass [67] in 1885, Hilbert [1893] in 1893, and many others. Lindemann in fact established more generally that

$$\beta_1 e^{\alpha_1} + \cdots + \beta_n e^{\alpha_n} \neq 0$$

for distinct algebraic numbers $\alpha_1, \ldots, \alpha_n$ and nonzero algebraic numbers $\beta_1, \ldots, \beta_n$. (See Exercise 7.) The transcendentality of π follows since $e^{i\pi} - 1 = 0$. This is the signal achievement of the nineteenth century with regard to transcendental number theory. Note that Lindemann's theorem implies the transcendence of $\cos\alpha$, $\sin\alpha$, and $\tan\alpha$ for algebraic $\alpha \neq 0$ and also the transcendence of $\log\beta$ for β algebraic, $\beta \neq 0$ or 1.

In 1900 Hilbert, as the seventh of his 23 problems posed at the International Congress in Paris, asked whether α^β is transcendental for α algebraic ($\alpha \neq 0, 1$) and β an algebraic irrational. This was solved independently by Gelfond and Schneider in 1934. (See Niven [56]). It is interesting to note that Hilbert had speculated that this problem would probably resist solution longer than the Riemann hypothesis or Fermat's last theorem. In 1966 Baker substantially generalized the Gelfond–Schneider theorem by showing

that any nonvanishing linear combination of logarithms of algebraic numbers with algebraic coefficients is transcendental. That is, if α_j and β_j are nonzero algebraic numbers, then $\beta_0 + \Sigma_{j=1}^{n} \alpha_j \log \beta_j \neq 0$. (See Baker [75].) Note that $i^i = e^{-\pi/2}$, and so transcendence of e^π follows from the Gelfond–Schneider theorem.

Comments and Exercises

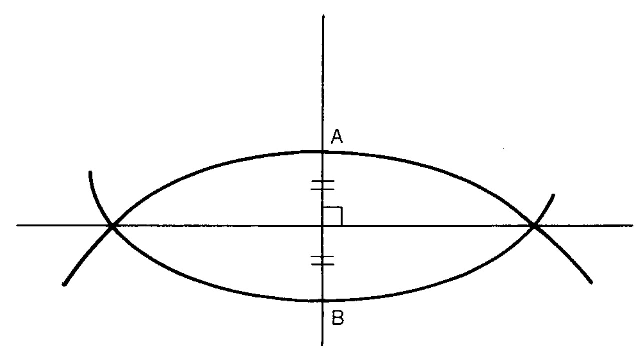
For a discussion of constructibility one might consult *Famous Problems in Elementary Geometry* by Klein [1897]. The treatment we give in Exercise 1 follows Clark [71]. The exercises on transcendental numbers follow Baker [75], Hardy and Wright [60], Hua [82], and LeVeque [77], and for the most part are simplifications of the original arguments. The particularly simple proof of the irrationality of π^2 (outlined in Exercise 3) is due to Niven [56]. The reader interested in pursuing these matters in depth is directed to Baker [75], Mahler [67], or Lang [66a].

1. (*On constructible numbers, doubling the cube, and trisecting the angle*) *Constructible numbers* can be defined by:

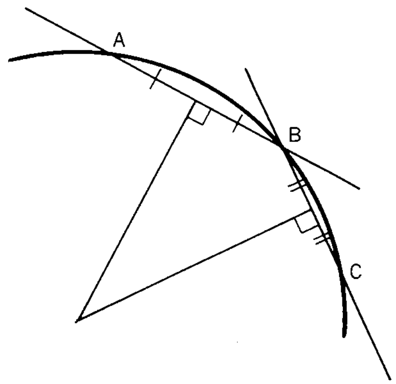
(i) The points $(0, 0)$ and $(0, 1)$ are constructible.
(ii) Lines joining constructible numbers are constructible.
(iii) Circles with constructible centers and constructible radii (that is, the radius is the distance between two constructible points) are constructible.
(iv) The points of intersection of constructible lines and circles are constructible.

It is the points of (iv) that form the constructible numbers.

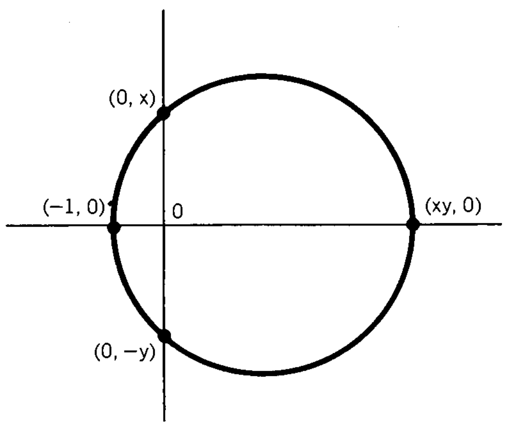
a) Prove that the constructible numbers are a subset of the algebraic numbers.
b) Show that perpendicular bisectors are constructible. See the hint provided in the illustration. *Hint*:



c) Show that a circle through three given points is constructible. See the hint provided in the illustration. *Hint*:



d) Show that the constructible numbers form a field. See the hint provided in the illustration. *Hint*:



e) A number field C is constructible if $C = \mathbb{Q}(c_1, \ldots, c_n)$, where $c_1, \ldots, c_n$ are all constructible. Show that if C is constructible, then C has degree 2^m over $\mathbb{Q}$.

f) Show that real extensions of degree 2 are constructible.

g) (*The impossibility of doubling the altar*) Use e) to show that $\sqrt[3]{2}$ is not construcible and so the Delian problem is not solvable.

h) (*The impossibility of trisecting the angle*) Show that constructing an angle θ is equivalent to constructing $\cos\theta$ and show that a 60° angle is constructible. Show that

$$\cos 3\theta = 4\cos^3\theta - 3\cos\theta$$

and hence, that $\cos 20°$ is a root of

$$8x^3 - 6x - 1.$$

Show that the above polynomial is irreducible over $\mathbb{Q}$ and hence, by part e), that a 20° angle is not constructible. Show that the constructibility of θ, given a rational $\cos 3\theta$, depends only on whether $4x^3 - 3x - \cos 3\theta$ factors over $\mathbb{Q}$. Show that a 30° angle is constructible.

The following series of exercises is on transcendental and algebraic numbers. Recall that α is *algebraic* of degree n if α is the root of an irreducible polynomial of degree n with integer coefficients. If α satisfies no such algebraic equation, it is *transcendental*.

2. (*On Liouville numbers*)

a) Prove that if α is algebraic of degree n, then for all $\varepsilon > 0$ and for all $c > 0$,

$$0 < \left|\alpha - \frac{p}{q}\right| < \frac{c}{q^{n+\varepsilon}}$$

has only finitely many solutions with p and q integral.
Hint: Suppose α satisfies

$$\rho(\alpha) := a_n\alpha^n + \cdots + a_0 = 0.$$

Then, provided p/q is not a root of ρ,

$$\left|\rho\left(\frac{p}{q}\right)\right| \geq \frac{1}{q^n}.$$

So by the mean value theorem, for $p/q \in [\alpha - 1, \alpha + 1]$,

$$\left|\alpha - \frac{p}{q}\right| \geq \frac{|\rho(\alpha) - \rho(p/q)|}{\sup\limits_{x\in[\alpha-1,\,\alpha+1]} |\dot{\rho}(x)|} > \frac{D}{q^n}$$

for some D, and the result follows.

A much deeper result of Roth (see Baker [75]) shows that a) holds with $q^{n+\varepsilon}$ replaced by $q^{2+\varepsilon}$.

b) Use a) to show that

$$\alpha := \sum_{n=1}^{\infty} \frac{1}{10^{n!}} \quad \text{and} \quad \beta := \sum_{n=1}^{\infty} \frac{1}{10^{2^{2^n}}}$$

are transcendental by showing that the partial sum approximations would violate a).

c) Modify the construction of b) to exhibit uncountably many transcendental numbers. (In fact, all infinite subseries of α are transcendental, which exhibits an uncountable set of such numbers.)

d) Show that the algebraic numbers are countable and hence, that almost all numbers are transcendental. Numbers that can be proved transcendental because they can be approximated too rapidly by rationals are called Liouville numbers. More precisely, α is a *Liouville number* if for every m there exists a rational p/q, $q>1$, so that

$$0<\left|\alpha-\frac{p}{q}\right|<\frac{1}{q^m}.$$

e) Prove that Liouvile numbers are transcendental.

f) Show that the set of Liouville numbers has measure zero.

g) Show that the Liouville numbers have Baire category II. Show, in fact, that the complement of the Liouville numbers is of Baire category I. Actually it is a nowhere dense F_σ. (Recall that a set is category I if it is the countable union of nowhere dense sets and that a set is nowhere dense if its closure has empty interior. A set is category II if it is not category I. See Oxtoby [80].)

3. (*On the irrationality of e and* π)

a) Prove that e is irrational.
Hint: Suppose $e=q/p$ and consider

$$\left|q!\left(\sum_{i=0}^{q}\frac{(-1)^i}{i!}-\frac{1}{e}\right)\right|.$$

Show that this is an integer strictly between 0 and 1.

b) Show that for any positive integer n,

$$f(x):=\frac{x^n(1-x)^n}{n!}$$

has the property that f and all its derivatives are integer valued at $x=0$ and $x=1$ and that for $x\in(0,1)$,

$$0<f(x)<\frac{1}{n!}.$$

c) Prove that e^p is irrational for integer $p\neq 0$.
Outline: Suppose $e^p=a/b$ with $a,b\in\mathbb{N}$. With f as in b), set

$$F(x):=p^{2n}f(x)-p^{2n-1}f^{(1)}(x)+\cdots+f^{(2n)}(x).$$

Show, by differentiating $e^{px}F(x)$, that

$$b\int_0^1 p^{2n+1}e^{px}f(x)\,dx=aF(1)-bF(0)$$

is an integer but that the left-hand side above lies strictly between 0 and 1 for large n.

d) Deduce from c) that e^q is irrational for all rational $q\neq 0$.

e) Show that π^2 (and hence π) is irrational.
Outline: Suppose $\pi^2=a/b$ with $a,b\in\mathbb{N}$. Let f be as in b) and consider

$$G(x):=b^n\sum_{k=0}^{n}(-1)^k f^{(2k)}(x)\pi^{2n-2k}.$$

Then

$$\frac{d}{dx}\{\dot G(x)\sin(\pi x)-\pi G(x)\cos(\pi x)\}=\pi^2a^nf(x)\sin(\pi x)$$

and

$$\pi\int_0^1 a^nf(x)\sin(\pi x)\,dx=G(0)+G(1).$$

However, $G(0)$ and $G(1)$ are integers while as in c) the integral on the left is strictly between 0 and 1 for large n.

4. (*On the transcendence of e*) This exercise outlines Hilbert's proof of the transcendence of e, a proof which, as LeVeque [77] puts it, is "as elegant as it is mysterious."

a) Recall that, for k an integer,

$$I_k:=\int_0^\infty x^ke^{-x}\,dx=k!$$

and thus if p is polynomial with integer coefficients,

$$\int_0^\infty x^kp(x)e^{-x}\,dx\equiv k!p(0)\bmod(k+1)!$$

b) Suppose e algebraic. Then there are integers a_i so that

$$a_0+a_1e+a_2e^2+\cdots+a_ne^n=0\qquad a_0\neq 0.$$

Let

$$\int_\alpha^\beta := \int_\alpha^\beta x^m[(x-1)\cdots(x-n)]^{m+1}e^{-x}\,dx$$

let

$$S := a_0\int_0^\infty + a_1 e\int_1^\infty + \cdots + a_n e^n\int_n^\infty$$

and let

$$T := a_1 e\int_0^1 + \cdots + a_n e^n \int_0^n .$$

Observe that $S + T = 0$.

c) Show that, for infinitely many m, $S/m!$ is a nonzero integer. To do this, observe that if $y := x - k$, then

$$a_k e^k \int_k^\infty = \begin{cases} a_0\int_0^\infty y^m p_0(y)e^{-y}\,dy & k=0\\ a_k\int_0^\infty y^{m+1}p_k(y)e^{-y}\,dy & k\ge 1\end{cases}$$

where the p_k are particular polynomials with integer coefficients. Now use a) to see that the first term of S is divisible by $m!$; that the rest are divisible by $(m+1)!$; and that for infinitely many m the first term is not divisible by $(m+1)!$.

d) Show that $\lim_{m\to\infty}|T|/m! = 0$. To do this let

$$M := \max_{0\le x\le n} |(x-1)(x-2)\cdots(x-n)|(x+1)$$

and show that

$$\left|a_k\int_0^k\right| \le k|a_k|M^{m+1}$$

whence

$$\frac{|T|}{m!} = O\left(\frac{M^{m+1}}{m!}\right) \to 0 .$$

e) Observe that, since $S + T = 0$, c) and d) lead to a contradiction, and hence e cannot be algebraic.

5. (*On the transcendence of* π) The exercise outlines Baker's [75] synthesis of Hilbert's proof of the transcendence of π.

a) Suppose $\theta_1 := i\pi$ is algebraic. Let l be the lead coefficient of the minimal polynomial for $i\pi$ and let $\theta_2, \ldots, \theta_d$ be the other roots of the minimal polynomial. Since $e^{i\pi} = -1$,

$$(1+e^{\theta_1})(1+e^{\theta_2})\cdots(1+e^{\theta_d}) = 0 .$$

Show that expanding the above yields a nonzero integer n such that

$$q + e^{\alpha_1} + \cdots + e^{\alpha_n} = 0$$

where $q := 2^d - n$ and each α_i is a nonzero sum of some subset of the θ_i of the form $\Sigma\,\delta_i\theta_i$, $\delta_i = 0$ or 1. Show that any elementary symmetric function of $l\alpha_1, \ldots, l\alpha_n$ with integer coefficients is integer valued. (See Exercise 6.)

b) Let

$$I(\alpha) := \int_0^\alpha e^{\alpha - t} f(t)\,dt$$

where

$$f(t) := l^{np}t^{p-1}(t-\alpha_1)^p\cdots(t-\alpha_n)^p$$

for some prime p. Let

$$J := I(\alpha_1) + \cdots + I(\alpha_n) .$$

Show, by using a) and repeated integration by parts, that for $m := (n+1)p - 1$,

$$J = -q\sum_{j=0}^m f^{(j)}(0) - \sum_{j=0}^m\sum_{k=1}^n f^{(j)}(\alpha_k) .$$

c) Show that J is an integer. To do this, observe that the right-hand term is a symmetric function of $l\alpha_1, \ldots, l\alpha_n$.

d) Show that for $j \ne p-1$,

$$p! \mid f^{(j)}(0)$$

while for $j = p - 1$,

$$f^{(p-1)}(0) = (p-1)!(-l)^{np}(\alpha_1\alpha_2\cdots\alpha_n)^p .$$

Thus for p sufficiently large,

$$(p-1)! \mid f^{(p-1)}(0) \quad \text{and} \quad p! \nmid f^{(p-1)}(0).$$

e) Show that, for $j \leq p-1$, and p sufficiently large

$$f^{(j)}(\alpha_k) = 0.$$

Show that

$$p! \Big| \sum_{j=0}^{m} \sum_{k=1}^{n} f^{(j)}(\alpha_k).$$

Hence with d)

$$|J| \geq (p-1)!$$

f) Show, however, that for some M independent of p,

$$|J| \leq |\Sigma I(\alpha_i)| \leq M^p.$$

This contradicts e) for large p and finishes the proof.

6. (*On symmetric polynomials*) A polynomial in n variables is *symmetric* if it remains unchanged by any permutation of the variables. An *elementary symmetric polynomial* f_i in the variables $x_1, \ldots, x_n$ is defined by

$$(y-x_1)(y-x_2)\cdots(y-x_n) = y^n - f_1 y^{n-1} + f_2 y^{n-2} - \cdots (-1)^n f_n.$$

a) Show by induction that any symmetric polynomial in n variables with integer coefficients can be written as a polynomial with integer coefficients in the elementary symmetric functions.

b) Let $s_k := x_1^k + \cdots + x_n^k$. Prove *Newton's identities*:

$$s_k = (-1)^{k+1} k f_k + (-1)^{k+1} \sum_{j=1}^{k-1} (-1)^j f_{k-j} s_j \qquad k \leq n$$

and

$$s_k = (-1)^{k+1} \sum_{j=k-n}^{k-1} (-1)^j f_{k-j} s_j \qquad k > n.$$

7. (*Lindemann's theorem*) This proof of Lindemann's theorem follows Baker [75] and assumes some general familiarity with algebraic integers. (An algebraic number whose minimal polynomial has lead coefficient 1: observe that if α is an algebraic number and the lead coefficient of the minimal polynomial is l, then $l\alpha$ is an algebraic integer.)

Lindemann's Theorem

If $\alpha_1, \ldots, \alpha_n$ are distinct algebraic numbers and $\beta_1, \ldots, \beta_n$ are nonzero algebraic numbers, then

$$\beta_1 e^{\alpha_1} + \cdots + \beta_n e^{\alpha_n} \neq 0.$$

a) Suppose that

$$\beta_1 e^{\alpha_1} + \cdots + \beta_n e^{\alpha_n} = 0.$$

Show that one can assume that

(i) The β_i are ordinary integers.
(ii) There exist integers $0 = n_0 < n_1 < \cdots < n_s = n$ so that, for each τ,

$$\alpha_{n_\tau+1}, \ldots, \alpha_{n_{\tau+1}}$$

is a complete set of conjugates and

$$\beta_{n_\tau+1} = \cdots = \beta_{n_{\tau+1}}.$$

b) Let l be an integer so that $l\alpha_1, \ldots, l\alpha_n$ and $l\beta_1, \ldots, l\beta_n$ are algebraic integers. For p a large prime, let

$$f_i(x) := \frac{l^{np}(x-\alpha_1)^p \cdots (x-\alpha_n)^p}{x-\alpha_i}.$$

For $1 \leq i \leq n$, let

$$J_i := \beta_1 I_i(\alpha_1) + \cdots + \beta_n I_i(\alpha_n)$$

where

$$I_i(\alpha) := \int_0^\alpha e^{\alpha - t} f_i(t)\, dt.$$

Show that

$$J_i = -\sum_{j=0}^{np-1} \sum_{k=1}^{n} \beta_k f_i^{(j)}(\alpha_k)$$

is an algebraic integer and that

$$(p-1)! \mid f_i^{(j)}(\alpha_k)$$

and for p sufficiently large

$$p! \nmid f_i^{(j)}(\alpha_k) \qquad j = p-1, \quad k = i$$

while

$$p! \mid f_i^{(j)}(\alpha_k) \qquad \text{otherwise}.$$

(An algebraic number α is divisible by h if α/h is an algebraic integer.)

c) Show that $|J_1 \cdots J_n|$ is a nonzero integer divisible by $(p-1)!$ and hence $|J_1 \cdots J_n| \geq (p-1)!$.

d) Show that there exists C independent of p so that

$$|J_1 \cdots J_n| = O(C^p)$$

and that this contradicts c).

8. (*Lengths and measures*)

a) Suppose P is a polynomial with integer coefficients of length L and degree D. Suppose α is an algebraic number with minimal polynomial of degree d and length l. (The *length* is the sum of the absolute value of the coefficients.) Show that either

$$P(\alpha) = 0$$

or

$$|P(\alpha)| \geq \frac{[\max(1, |\alpha|)]^D}{L^{d-1} l^D} \geq \frac{1}{L^{d-1} l^D}.$$

Hint: Suppose $\alpha_1 := \alpha$ has minimal polynomial

$$Q(x) := q_d x^d + \cdots + q_0$$

and let $\alpha_2, \ldots, \alpha_d$ be the remaining roots of Q. Show that

$$q_d^D \cdot P(\alpha_1) P(\alpha_2) \cdots P(\alpha_d)$$

is a nonzero integer [if $P(\alpha_1) \neq 0$]. Since

$$|P(\alpha_k)| \leq L \cdot \max(1, |\alpha_k|)^D$$

we have

$$1 \leq |q_d^D| \, |P(\alpha_1)| \prod_{k=2}^{d} [L \max(1, |\alpha_k|)^D]$$
$$\leq l^D L^{d-1} \max(1, |\alpha_1|)^{-D} |P(\alpha_1)|$$

where the last inequality requires showing

$$l \geq |q_d| \prod_{k=1}^{d} \max(1, |\alpha_k|)$$

and follows from part b) of this exercise.

b) Let P and Q be polynomials and let

$$\mu(P) := \exp\left[\int_0^1 \log|P(e^{2\pi i t})|\, dt\right].$$

Show that

i) $\mu(PQ) = \mu(P)\mu(Q)$

ii) $\mu(P) \leq \text{length } (P)$

iii) $\mu(x - c) = \mu(x - |c|)$

iv) $\mu((x - c^n)^{1/n}) = \mu(x - c)$

v) $\mu(x - c) = \max(1, |c|)$

vi) $\mu\left(c \prod_{i=1}^{n} (x - \alpha_i)\right) = |c| \prod_{i=1}^{n} \max(1, |\alpha_i|)$.

(μ is called the *measure* of P.)

The next exercise constructs a form

$$p_n(x) e^{nx} + \cdots + p_1(x) e^x + p_0(x) = O(x^{(n+1)(m+1)-1})$$

where the p_i are polynomials of degree $\leq m$ with integer coefficients. Such forms can be viewed as higher dimensional Padé approximants. Setting $x := 1$ in the above leads to a polynomial in e that can, in conjunction with Exercise 8, be used to prove the transcendence of e. Setting $x := i\pi$, so that $e^{i\pi} = -1$, leads to a proof of the transcendence of π. Such forms were examined by Hermite. It was, however, Mahler [31] who showed how to base the transcendence proofs on them.

9. (*Another proof of the transcendance of e and π*)

a) Suppose that we can find V_n so that

$$V_{n,m} := V_n := p_n e^{nx} + \cdots + p_1 e^x + p_0 = O(x^{(n+1)(m+1)-1})$$

where each p_i is of degree m and $p_n := x^m + \cdots$. Then

$$V_n^{(m+1)} = s_n e^{nx} + \cdots + s_1 e^x = O(x^{n(m+1)-1})$$

where each s_i is of degree m. In particular

$$V_n^{(m+1)} = n^{m+1} V_{n-1} e^x$$

and

$$V_1^{(m+1)} = x^m e^x .$$

b) Prove that, for sufficiently smooth G, if

$$G(x) := \frac{1}{m!} \int_0^x (x-t)^m f(t)\, dt$$

then $G^{(m+1)}(x) = f(x)$. Use this to show that

$$\begin{aligned} V_n &= \frac{(n)^{m+1}}{m!} \int_0^x (x-t)^m V_{n-1}(t) e^t\, dt \\ &= \frac{(n!)^{m+1}}{(m!)^n} \int_0^x \int_0^{t_1} \int_0^{t_2} \cdots \int_0^{t_{n-1}} (x-t_1)^m (t_1 - t_2)^m \cdots (t_{n-1} - t_n)^m t_n^m \\ &\quad \times e^{t_1 + t_2 + \cdots + t_n}\, dt_n \cdots dt_1 . \end{aligned}$$

c) Thus

$$V_{n,m} = \frac{(n!)^{m+1}}{(m!)^n} x^{(n+1)(m+1)-1} \overline{\int_0^1} M(x)\, d\bar{t}$$

where

$$\overline{\int_0^1} d\bar{t} := \int_0^1 \cdots \int_0^1 \int_0^1 dt_n \cdots dt_1$$

and where

$$\begin{aligned} M(x) := {} & [(1-t_1)\cdots(1-t_n)]^m t_n^m t_{n-1}^{2m+1} t_{n-2}^{3m+2} \cdots t_1^{nm+n-1} \\ & \times e^{t_1 x} e^{t_1 t_2 x} e^{t_1 t_2 t_3 x} \cdots e^{t_1 t_2 \cdots t_n x} . \end{aligned}$$

d) Use c) to show that $V_{n,m}$, defined as in a), exists and is uniquely defined for all m and n.

e) Show that if C_δ is a circle of radius $\delta > n$, then

$$V_{n,m} = \frac{m!(n!)^{m+1}}{2\pi i} \int_{C_\delta} \frac{e^{tx}\, dt}{[t(t-1)\cdots(t-n)]^{m+1}} .$$

Hint: Use the residue theorem to see that $V_{n,m}$ is of the right form.

Observe by expanding e^{tx} and evaluating on circles of large radius that

$$V_{n,m} = O(x^{(n+1)(m+1)-1}) .$$

f) Show that, with $\delta < 1$,

$$p_k(x) = \frac{m!(n!)^{m+1}}{2\pi i} \int_{C_\delta} \frac{e^{tx}\, dt}{[\prod_{i=0}^n (t+k-i)]^{m+1}} .$$

Hint: Show by the residue theorem that p_k is a polynomial of degree m and that, with e),

$$\sum_{k=0}^n p_k e^{kx} = V_{n,m} .$$

Note that

$$p_k(x) = (n!)^{m+1} \left[\frac{d}{dt}\right]^m \left(\frac{e^{tx}}{\prod_{\substack{i=0 \\ i \neq k}}^n (t+k-i)^{m+1}} \right) \Bigg|_{t=0} .$$

The $n := 1$ case of e) and f) provides an alternate derivation of the Padé approximant, equation (10.1.15).

g) Use f) to show that

$$d_n^m p_k$$

has integer coefficients [$d_n := \mathrm{LCM}(1, \ldots, n)$].

h) Let n be fixed. Show from c) that for m sufficiently large,

$$V_n(x) \neq 0 \qquad \text{for } x \neq 0 .$$

Note that this is trivial for real $x \neq 0$.

i) Let $D > e$ and let

$$W_{n,m}(x) := d_n^m V_{n,m}(x) .$$

From c) show that

$$W_{n,m}(x) = \sum_{\substack{0 \le k \le n \\ 0 \le j \le m}} a_{kj} x^j e^{kx}$$

where the a_{kj} are integers. Use c) and the fact that $d_n < e^{n(1+\varepsilon)}$ for large n (Exercise 6 of Section 11.3) to show that for $m+n$ large,

$$|W_{m,n}(x)| \le \frac{|x|^{(n+1)(m+1)-1} e^{n|x|} D^{nm} (n!)^{m+1} m!}{[(n+1)(m+1)-1]!} .$$

Show from f) with $\delta := 1/n$, that for $m+n$ large,

$$|a_{kj}| \le \frac{n^{2(m+1)} D^{nm} (m!) 2^{n(m+1)}}{(n-1)^{m+1}}.$$

j) Let $x \neq 0$ and n be fixed. Then for m sufficiently large,

$$0 < |W_{n,m}(x)| \le \frac{c_1^{nm}}{m^{nm}}$$

and

$$|a_{kj}| \le c_2^{nm} m^m$$

where c_1 and c_2 are constants, independent of n and m.

k) Show that e is transcendental.
Hint: Let $P_m(e) = W_{n,m}(1)$ for fixed large n. Show that as $m \to \infty$, $P_m(e)$ is sufficiently small that, by Exercise 8, e must be transcendental.

l) Show that π is transcendental.
Hint: Let $x := i\pi$ in i) so that $e^{i\pi} = -1$. Now proceed as in k). Observe that $W_{n,m}(i\pi)$ is a polynomial of degree m in π.

11.3 *IRRATIONALITY MEASURES*

We examine the rate of approximation of e, π, and $\log 2$ by rationals. For example, we show, for p and q integers and q sufficiently large, that

$$\left|\pi - \frac{p}{q}\right| > \frac{1}{q^{24}}. \tag{11.3.1}$$

Estimates such as (11.3.1) are termed *irrationality measures*. The expected rate of rational approximation is as follows: If $f(x)$ is a positive nonincreasing function, then

$$\left|\alpha - \frac{p}{q}\right| < \frac{f(q)}{q} \tag{11.3.2}$$

has infinitely many integer solutions in p and q for almost all α exactly when

$$\sum_{q=1}^{\infty} f(q) = \infty. \tag{11.3.3}$$

Thus, with probability 1, we expect

$$\left|\alpha - \frac{p}{q}\right| < \frac{1}{q^2 \log q} \tag{11.3.4}$$

to have infinitely many solutions, while

$$\left|\alpha - \frac{p}{q}\right| < \frac{1}{q^2 (\log q)^{1+}} \tag{11.3.5}$$

← omitted

usually has only finitely many solutions. This result is due to Khinchin [64]. (See also Exercise 2 of Section 11.2 and Exercise 1 of this section.)

It is standard to the theory of continued fractions that if

$$\left|\alpha - \frac{p}{q}\right| < \frac{1}{2q^2} \qquad p, q \in \mathbb{Z} \tag{11.3.6}$$

then p/q is a convergent of the simple continued fraction for α, while of any two consecutive convergents of the continued fraction, at least one of them satisfies (11.3.6). (See Exercise 2.) Roth's theorem states that for algebraic α,

$$\left|\alpha - \frac{p}{q}\right| < \frac{1}{q^{2+\varepsilon}} \qquad \varepsilon > 0 \tag{11.3.7}$$

has at most finitely many solutions. (See Baker [75].)

For specific transcendentals exact estimates are usually unknown, but e can be analyzed very precisely.

Theorem 11.1

If

$$s_n := \sum_{k=0}^{n} \frac{(2n-k)!}{(n-k)!k!} \qquad t_n := \sum_{k=0}^{n} \frac{(2n-k)!}{(n-k)!k!} (-1)^k \tag{11.3.8}$$

then

$$\left|e - \frac{s_n}{t_n}\right| = \frac{1}{2} \frac{\log\log t_n}{t_n^2 \log t_n} [1 + o(1)]. \tag{11.3.9}$$

Proof. From Exercise 10 of Section 10.1, with $s_n := P_{n,n}(1)$ and $t_n := Q_{n,n}(1)$ we have

$$\left|e - \frac{s_n}{t_n}\right| = \frac{n!n!}{(2n)!(2n+1)!} e[1 + o(1)] \tag{11.3.10}$$

and

$$t_n = \frac{(2n)!}{n!} e^{-1/2}[1 + o(1)]. \tag{11.3.11}$$

The result now follows, as an application of Stirling's formula gives

$$2n + 1 = \frac{2 \log t_n}{\log \log t_n} [1 + o(1)]. \quad \square \tag{11.3.12}$$

Theorem 11.2

If $p, q \in \mathbb{Z}$ and

$$\left|e - \frac{p}{q}\right| < \frac{1}{4q^2}$$

then, for some n, $p/q = s_n/t_n$, where s_n and t_n are as in Lemma 11.1.

Proof. The continued fraction for $(e-1)/2$ is given by

$$\frac{e-1}{2} = [0, 1, 6, 10, 14, 18, \ldots] := [a_0, a_1, \ldots]. \tag{11.3.13}$$

If $p_n := (s_n - t_n)/2$ and $q_n := t_n$, then one can verify that

$$p_n = a_n p_{n-1} + p_{n-2} \qquad p_0 = 0 \qquad p_1 = 1 \tag{11.3.14}$$

$$q_n = a_n q_{n-1} + q_{n-2} \qquad q_0 = 1 \qquad q_1 = 1. \tag{11.3.15}$$

This, with Theorem 11.1, shows that p_n/q_n are the convergents for the simple continued fraction for $(e-1)/2$ and that expansion (11.3.13) holds. (See Exercise 2.) In particular, if

$$\left|e - \frac{p}{q}\right| < \frac{1}{4q^2} \quad \text{then} \quad \left|\frac{e-1}{2} - \frac{p-q}{2q}\right| < \frac{1}{8q^2}$$

and by Exercise 2i), $(p-q)/2q$ is a convergent of (11.3.13). $\square$

Corollary 11.1

Let $0 < \delta < 1$ and let v be a positive integer. Then

$$\left|e^{1/v} - \frac{p}{q}\right| \le \frac{1+\delta}{2v} \frac{\log \log q}{q^2 \log q} \tag{11.3.16}$$

has infinitely many integer solutions, while

$$\left|e^{1/v} - \frac{p}{q}\right| \le \frac{1-\delta}{2v} \frac{\log \log q}{q^2 \log q} \tag{11.3.17}$$

has at most finitely many integer solutions.

The above corollary due to Davis [79] shows that $e^{1/v}$ is atypical with respect to the rate of rational approximation [compare (11.3.4) and (11.3.5)]. For $v = 1$, Corollary 11.1 can be deduced from Theorem 11.1 without reference to Theorem 11.2 on continued fractions. (See Exercise 4.) For general v the proof is left as Exercise 5.

We now turn to irrationality measures for π, $\zeta(2)$, and $\zeta(3)$. The approach follows Beuker's [79] elegant treatment of Apéry's startling proof of the irrationality of $\zeta(3)$.

Lemma 11.1

Let r and s be nonnegative integers.

(a) $$\int_0^1 \int_0^1 \frac{x^r y^s \, dx\, dy}{1-xy} = \begin{cases} \dfrac{n}{d_r^2} \quad \text{for some } n \text{ in } \mathbb{Z} & r > s \\ \zeta(2) - \dfrac{1}{1^2} - \dfrac{1}{2^2} - \cdots - \dfrac{1}{r^2} & r = s > 0 \\ \zeta(2) & r = s = 0 \end{cases}$$

(b) $$\int_0^1 \int_0^1 \frac{-x^r y^s \log xy \, dx\, dy}{1-xy} = \begin{cases} \dfrac{n}{d_r^3} \quad \text{for some } n \text{ in } \mathbb{Z} & r > s \\ 2\left[\zeta(3) - \dfrac{1}{1^3} - \dfrac{1}{2^3} - \cdots - \dfrac{1}{r^3}\right] & r = s > 0 \\ 2\zeta(3) & r = s = 0 \end{cases}$$

where $d_r := \mathrm{LCM}(1, 2, \ldots, r)$.

Proof. Consider

$$I := \int_0^1 \int_0^1 \frac{x^{r+\delta} y^{s+\delta}}{1-xy} \, dx\, dy. \tag{11.3.18}$$

If we expand $(1-xy)^{-1}$ and integrate term by term, we get

$$I = \sum_{k=0}^{\infty} \frac{1}{(k+r+\delta+1)(k+s+\delta+1)} \tag{11.3.19}$$

which on setting $\delta = 0$ establishes the $r = s$ case of (a). For $r > s$,

$$I = \sum_{k=0}^{\infty} \frac{1}{r-s}\left[\frac{1}{k+s+\delta+1} - \frac{1}{k+r+\delta+1}\right]$$

$$= \frac{1}{r-s}\left[\frac{1}{s+1+\delta} + \cdots + \frac{1}{r+\delta}\right] \tag{11.3.20}$$

which establishes the rest of (a). If we differentiate I with respect to δ and set $\delta = 0$, we get

$$\int_0^1 \int_0^1 \frac{x^r y^s \log xy}{1-xy}\, dx\, dy \tag{11.3.21}$$

and part (b) follows from differentiating (11.3.19) and (11.3.20). □

Theorem 11.3

$\zeta(2) = \pi^2/6$ is irrational.

Proof. Let p_n be the "shifted" Legendre polynomial

$$p_n(x) := \frac{1}{n!}\left\{\frac{d}{dx}\right\}^n x^n(1-x)^n \tag{11.3.22}$$

and note that

$$p_n(x) = \sum_{k=0}^{n} \binom{n}{k} \frac{(n+k)!}{n!k!}(-1)^k x^k \tag{11.3.23}$$

is a polynomial of degree n with integer coefficients. Consider

$$\begin{aligned} I_n &:= \int_0^1 \int_0^1 \frac{(1-y)^n p_n(x)}{1-xy}\, dx\, dy \\ &= (-1)^n \int_0^1 \int_0^1 \frac{y^n(1-y)^n x^n(1-x)^n}{(1-xy)^{n+1}}\, dx\, dy \end{aligned} \tag{11.3.24}$$

where the equality follows on integrating n times by parts with respect to x. Since for $0 \le x, y \le 1$,

$$\frac{xy(1-y)(1-x)}{1-xy} \le \left(\frac{\sqrt{5}-1}{2}\right)^5 \tag{11.3.25}$$

[with equality for $x = y = (\sqrt{5}-1)/2$] we have, by (11.3.24) and Lemma 11.1(a),

$$0 < |I_n| \le \left(\frac{\sqrt{5}-1}{2}\right)^{5n} \zeta(2). \tag{11.3.26}$$

On the other hand by the same lemma applied to the first form of I_n,

$$|I_n| = \left|\beta_n \zeta(2) - \frac{\alpha_n}{d_n^2}\right| \tag{11.3.27}$$

where

$$\beta_n = \sum_{k=0}^{n} \binom{n}{k}\binom{n}{k} \frac{(n+k)!}{n!k!}, \tag{11.3.28}$$

α_n is an integer and $d_n = \mathrm{LCM}(1, 2, \ldots, n)$. It is a simple consequence of the prime number theorem (see Exercise 6) that, for any $\eta > 1$,

$$d_n = O(e^{\eta n}). \tag{11.3.29}$$

Furthermore, Stirling's formula and a little calculus lead to the estimate

$$c_1 n^{c_2}\left(\frac{1+\sqrt{5}}{2}\right)^{5n} \le \beta_n \le c_3 n^{c_4}\left(\frac{1+\sqrt{5}}{2}\right)^{5n} \tag{11.3.30}$$

where $c_1 > 0$, c_2, c_3, and c_4 are constants. In fact, van der Poorten [79] gives

$$\beta_n = \frac{[(1+\sqrt{5})/2]^4}{2\pi\sqrt{5+2\sqrt{5}}} \frac{[(1+\sqrt{5})/2]^{5n}}{n}\left[1 + O\left(\frac{1}{n}\right)\right].$$

From (11.3.26), (11.3.27), (11.3.29), and (11.3.30) we deduce that for sufficiently large n,

$$0 < \left|\zeta(2) - \frac{\alpha_n}{\gamma_n}\right| \le \frac{1}{\gamma_n^{1+\delta+}} \tag{11.3.31}$$

where $\gamma_n := d_n^2 \beta_n$ and α_n are integers, and where

$$\delta := \frac{\log[(1+\sqrt{5})/(\sqrt{5}-1)]^5}{\log\{[(1+\sqrt{5})/2]^5 e^2\}} - 1 = 0.092159\ldots > 0. \tag{11.3.32}$$

Thus (11.3.31) proves the irrationality of $\zeta(2) = \pi^2/6$. □

Theorem 11.4

For p and q integers and q sufficiently large,

$$\left|\pi^2 - \frac{p}{q}\right| > \frac{1}{q^{11.86}} \tag{11.3.33}$$

and

$$\left|\pi - \frac{p}{q}\right| > \frac{1}{q^{23.72}}. \tag{11.3.34}$$

Proof. From (11.3.30), (11.3.31), (11.3.32), and Exercise 3 we deduce that, given $\varepsilon > 0$, if

$$\left|\frac{\pi^2}{6} - \frac{p}{q}\right| < \frac{1}{q^{1+1/\delta+\varepsilon}}$$

for sufficiently large q, then $p/q = \alpha_n/\gamma_n$ for some n. [Here α_n, γ_n, and $\delta := 0.092\ldots$ are as in (11.3.31).] Thus we need only verify (11.3.33) for $p/q = \alpha_n/\gamma_n$. This follows from the observation that, for small $\eta > 0$ and for large n,

$$I_n > \left(\frac{\sqrt{5}-1}{2} - \eta\right)^{5n}.$$

[See (11.3.24) and (11.3.25).] In conjunction with (11.3.27) this leads to

$$\left|\zeta(2) - \frac{\alpha_n}{\gamma_n}\right| \geq \frac{[(\sqrt{5}-1)/2 - \eta]^{5n}}{\gamma_n}.$$

One now finishes the result by using estimates (11.3.29) and (11.3.30) to show that

$$\frac{[(\sqrt{5}-1)/2 - \eta]^{5n}}{\gamma_n} \geq \frac{1}{\gamma_n^3} > \frac{1}{\gamma_n^{11.86}}$$

for large n and small η.

The irrationality measure for π follows from the irrationality measure for π^2 since, for large q,

$$\left|\pi - \frac{p}{q}\right| = \frac{1}{|\pi + p/q|}\left|\pi^2 - \frac{p^2}{q^2}\right| > \frac{1}{|\pi + p/q|}\,\frac{1}{q^{2\cdot 11.86\ldots}}. \quad \square$$

The first irrationality measure for π was due to Mahler [53] (see also Mahler [67]), who showed that

$$\left|\pi - \frac{p}{q}\right| > \frac{1}{q^{42}} \qquad q \geq 2.$$

This was later refined by Mignotte [74] to

$$\left|\pi - \frac{p}{q}\right| > \frac{1}{q^{20.6}} \qquad q \geq 2$$

and by Chudnovsky and Chudnovsky [84] to

$$\left|\pi - \frac{p}{q}\right| > \frac{1}{q^{14.65}} \qquad q \text{ large}$$

(which can be marginally sharpened).

Theorem 11.5

$\zeta(3)$ is irrational.

Proof. Consider

$$I_n := \int_0^1\int_0^1 \frac{-\log xy}{1-xy}\, p_n(x)p_n(y)\,dx\,dy \tag{11.3.35}$$

where, as in (11.3.22),

$$p_n(x) = \frac{1}{n!}\left\{\frac{d}{dx}\right\}^n x^n(1-x)^n.$$

We observe that

$$\frac{-\log xy}{1-xy} = \int_0^1 \frac{1}{1-(1-xy)z}\,dz$$

and rewrite (11.3.35) as

$$I_n = \int_0^1\int_0^1\int_0^1 \frac{p_n(x)p_n(y)}{1-(1-xy)z}\,dx\,dy\,dz.$$

An n-fold integration by parts with respect to x yields

$$I_n = \int_0^1\int_0^1\int_0^1 \frac{(xyz)^n(1-x)^n p_n(y)}{[1-(1-xy)z]^{n+1}}\,dx\,dy\,dz$$

which, on substituting $w := (1-z)/[1-(1-xy)z]$, becomes

$$\begin{aligned} I_n &= \int_0^1\int_0^1\int_0^1 \frac{(1-x)^n(1-w)^n p_n(y)}{1-(1-xy)w}\,dx\,dy\,dw \\ &= \int_0^1\int_0^1\int_0^1 \frac{[x(1-x)w(1-w)y(1-y)]^n}{[1-(1-xy)w]^{n+1}}\,dx\,dy\,dw \end{aligned} \tag{11.3.36}$$

where the last equality follows from an n-fold integration by parts with respect to y. For $0 \leq x, y, w \leq 1$,

$$\frac{x(1-x)w(1-w)y(1-y)}{1-(1-xy)w} \leq (\sqrt{2}-1)^4$$

and from (11.3.36),

$$0 < I_n \leq 2\zeta(3)(\sqrt{2}-1)^{4n}. \tag{11.3.37}$$

From Lemma 11.1(*b*),

(11.3.38) $$I_n = \left|\beta_n' \zeta(3) - \frac{\alpha_n'}{d_n^3}\right|$$

where α_n', β_n', and d_n^3 are integers. Since $e^3(\sqrt{2}-1)^4 < 1$ and β_n' grows at most geometrically [see (11.3.42)], we deduce that there exists $\delta' > 0$ so that

(11.3.39) $$0 < \left|\zeta(3) - \frac{\alpha_n'}{\beta_n' d_n^3}\right| \le \frac{1}{(\beta_n' d_n^3)^{1+\delta'}}$$

for large n. This proves the irrationality of $\zeta(3)$. □

Corollary 11.2

For p and q integers and q sufficiently large,

(11.3.40) $$\left|\zeta(3) - \frac{p}{q}\right| > \frac{1}{q^{13.42}}.$$

Proof. The proof is similar to the proof of Theorem 11.3 and 11.4. One first calculates β_n' explicitly from (11.3.35) and (11.3.23),

(11.3.41) $$\beta_n' = 2\sum_{k=0}^{n} \binom{n}{k}^2 \binom{n+k}{n}^2.$$

From Stirling's formula one can show that

(11.3.42) $$c_1 n^{c_2}(1+\sqrt{2})^{4n} \le \beta_n' \le c_3 n^{c_4}(1+\sqrt{2})^{4n}$$

for constants $c_1 > 0$, c_2, c_3, and c_4. In fact,

(11.3.43) $$\beta_n' = \frac{2(1+\sqrt{2})^2}{n^{3/2}(2\pi\sqrt{2})^{3/2}}(1+\sqrt{2})^{4n}\left[1 + O\left(\frac{1}{n}\right)\right].$$

The remainder of the proof follows much as in Theorem 11.4, and the details are left as Exercise 8. □

Similar considerations lead to the irrationality measures for log.

Theorem 11.6

Let p, q, and n be integers. Then

(11.3.44) $$\left|\log 2 - \frac{p}{q}\right| > \frac{1}{q^{4.63}} \qquad q \text{ large}$$

and for any $\varepsilon > 0$, and fixed $n > N_\varepsilon$

(11.3.45) $$\left|\log\frac{n+1}{n} - \frac{p}{q}\right| > \frac{1}{q^{2+\varepsilon}} \qquad q \text{ large}.$$

The proof of the theorem is sketched in Exercise 9 or in Alladi and Robinson [79]. Similar results may be found in Baker [75]. The best known irrationality estimate for log 2 is also due to Chudnovsky and Chudnovsky [84], who show that the constant can be reduced to 4.13... in (11.3.44).

Comments and Exercises

Results on the rational approximation of e may be found in Adams [66], Bundschuh [71], and Davis [79]. Adams shows that the number of relatively prime integer solutions of

$$\left|e - \frac{p}{q}\right| < \frac{1}{q^2} \qquad \text{and} \qquad 1 < q < n$$

behaves like $3\log n/(\log\log n)$ (rather than the expected $c\log n$ that holds for almost all numbers).

Transcendence estimates of type

(11.3.46) $$|\pi - \beta| > \frac{1}{h^{cd\log d}} \qquad h \text{ large}$$

where β is an algebraic number of degree d and height h (the *height* is the modulus of the maximum coefficient of the minimal polynomial) due to Feldman are discussed in Baker [75].

Irrationality measures are often difficult. The best known estimate for e^π is

$$\left|e^\pi - \frac{p}{q}\right| > \frac{1}{q^{c\log\log q}} \qquad c \text{ a constant}.$$

Apéry's proof of the irrationality of $\zeta(3)$ does not obviously extend to other values of ζ. It is not known whether $\zeta(2n+1)$ is irrational for $n > 1$. Equally, whether $(\log\pi)/\pi$, $e+\pi$, Catalan's constant, and Euler's constant are irrational is unknown.

1. Let f be a positive nonincreasing function so that

$$\sum_{q=1}^{\infty} f(q) < \infty.$$

Show that the set of α for which

$$\left|\alpha - \frac{p}{q}\right| < \frac{f(q)}{q}$$

has infinitely many solutions has (Lebesque) measure zero. (The other half of Khinchin's theorem is more delicate.)

Hint: Fix N. For each $q > N$ consider intervals of radius $f(q)/q$ around the q points $0/q, 1/q, \ldots, (q-1)/q$. The measure of the union of all these intervals is bounded by

$$\sum_{q \geq N} q \frac{2f(q)}{q}.$$

2. (*On simple continued fractions*) For integral a_i, $a_0 \geq 0$, $a_i > 0$, $i \neq 0$, let

$$[a_0, a_1, \ldots, a_n] := a_0 + \cfrac{1}{a_1 + \cfrac{1}{a_2 + \cfrac{1}{a_3 + \ddots + \cfrac{1}{a_n}}}}$$

and let

$$[a_0, a_1, \ldots] := \lim_{n \to \infty} [a_0, a_1, \ldots, a_n].$$

Unless otherwise specified, we assume the continued fraction is infinite. The *nth convergent* is defined by

$$\frac{p_n}{q_n} := [a_0, a_1, \ldots, a_n].$$

a) Show that the convergents satisfy

$$\text{(11.3.47)} \qquad p_n = a_n p_{n-1} + p_{n-2} \qquad p_1 = a_1 a_0 + 1 \qquad p_0 = a_0$$

$$\text{(11.3.48)} \qquad q_n = a_n q_{n-1} + q_{n-2} \qquad q_1 = a_1 \qquad q_0 = 1$$

$$\text{(11.3.49)} \qquad p_n q_{n-1} - p_{n-1} q_n = (-1)^{n-1}$$

$$\text{(11.3.50)} \qquad p_n q_{n-2} - p_{n-2} q_n = (-1)^n a_n$$

$$\text{(11.3.51)} \qquad \frac{p_{2n}}{q_{2n}} \geq \frac{p_{2n-2}}{q_{2n-2}} \qquad \frac{p_{2n+1}}{q_{2n+1}} \leq \frac{p_{2n-1}}{q_{2n-1}}.$$

Deduce that p_n and q_n are relatively prime. Note that $\{p_n\}$ and $\{q_n\}$ are increasing sequences.

b) Show that continued fractions are well defined, that is, show that the limit in the definition always exists.

c) Rational numbers have two representations since

$$[a_0, \ldots, a_n] = [a_0, \ldots, a_{n-1} + 1] \qquad a_n = 1$$

and

$$[a_0, \ldots, a_n] = [a_0, \ldots, a_{n-1}, a_n - 1, 1] \qquad a_n \neq 1.$$

Show that a number is rational if and only if it has a finite simple continued fraction. [See e).]

d) Let $\alpha_n' := [a_n, a_{n+1}, \ldots]$ where $\alpha := [a_0, a_1, \ldots]$. Show that

$$\alpha - \frac{p_n}{q_n} = \frac{(-1)^n}{q_n(\alpha_{n+1}' q_n + q_{n-1})}.$$

Thus $\{p_{2n}/q_{2n}\} \uparrow \alpha$ and $\{p_{2n+1}/q_{2n+1}\} \downarrow \alpha$.

e) One constructs the simple continued fraction to α as follows ($\lfloor\ \rfloor :=$ integer part). Let

$$a_0 := \lfloor \alpha \rfloor \qquad \text{and} \qquad \alpha_0 := \alpha$$

and proceed inductively to let

$$\alpha_{n+1} := \frac{1}{\alpha_n - \lfloor \alpha_n \rfloor} \qquad \text{and} \qquad a_{n+1} := \lfloor \alpha_{n+1} \rfloor$$

unless $\alpha_n - \lfloor \alpha_n \rfloor = 0$, in which case the algorithm terminates. Show that

$$\alpha = [a_0, a_1, \ldots]$$

and if the continued fraction is infinite, then the representation is unique.

f) Show from d) that

$$\left| \alpha - \frac{p_n}{q_n} \right| < \frac{1}{q_n q_{n+1}} < \frac{1}{q_n^2}.$$

g) (*Best approximation property*) Show that if $0 < q < q_n$ and if $p/q \neq p_n/q_n$, then

$$\left| \frac{p_n}{q_n} - \alpha \right| < \left| \frac{p}{q} - \alpha \right|.$$

Hint: Prove $|p_n - q_n \alpha| < |p - q\alpha|$. Show first that one may assume $q_{n-1} < q < q_n$. Now write $q := uq_n + vq_{n-1}$, $p := up_n + vp_{n-1}$, and $p_n - q_n \alpha = u(p_n - q_n \alpha) + v(p_{n-1} - q_{n-1}\alpha)$. Show that u and v are nonzero integers and that $u(p_n - q_n\alpha)$ and $v(p_{n-1} - q_{n-1}\alpha)$ have the same sign.

h) Show that if for $z > 1$,

$$\alpha = \frac{pz + r}{qz + s} \qquad p, q, r, s \in \mathbb{Z}$$

and

$$q > s > 0 \qquad ps - qr = \pm 1$$

then r/s and p/q are consecutive convergents of the continued fraction for α.
Hint: Write p/q as a continued fraction and show that if

$$\frac{p}{q} = [a_0, \ldots, a_n]$$

then

$$\alpha = [a_0, \ldots, a_n, z] \qquad \text{and} \qquad z = [a_{n+1}, a_{n+2}, \ldots].$$

[There are two representations for p/q [part c)]. Choose the one for which n satisfies $ps - qr = (-1)^{n-1}$.]

i) Show that if

$$\left|\alpha - \frac{p}{q}\right| < \frac{1}{2q^2}$$

then p/q is a convergent of α.
Hint: Suppose

$$\frac{p}{q} - \alpha = \frac{(-1)^{n-1}\delta}{q^2} \qquad 0 < \delta < \frac{1}{2}$$

and

$$\frac{p}{q} = [a_0, a_1, \ldots, a_n].$$

Write

$$\alpha = \frac{p_n z + p_{n-1}}{q_n z + q_{n-1}}$$

where p_i/q_i is the ith convergent to p/q. Show that $z > 1$ and apply h).

j) Of two consecutive convergents at least one satisfies

$$\left|\alpha - \frac{p_n}{q_n}\right| < \frac{1}{2q_n^2}.$$

Hint: By a), if the above fails, then

$$\frac{1}{q_n q_{n+1}} = \left|\frac{p_{n+1}}{q_{n+1}} - \frac{p_n}{q_n}\right| = \left|\frac{p_n}{q_n} - \alpha\right| + \left|\frac{p_{n+1}}{q_{n+1}} - \alpha\right| \geq \frac{1}{2q_n^2} + \frac{1}{2q_{n+1}^2}.$$

Hurwitz has shown that of any three consecutive convergents at least one satisfies

$$\left|\alpha - \frac{p_n}{q_n}\right| < \frac{1}{\sqrt{5}q^2}.$$

This cannot be sharpened since, for example,

$$\left|\frac{\sqrt{5}-1}{2} - \frac{p}{q}\right| \geq \frac{1}{(\sqrt{5}-\delta)q^2} \qquad \delta > 0$$

for q sufficiently large. (See, for example, Hua [82].)

k) (*Fibonacci numbers*) Let

$$F_{n+1} := F_n + F_{n-1} \qquad F_1 := F_0 := 1.$$

Show that $\{F_{n+1}/F_n\}$ are the convergents to $(1+\sqrt{5})/2$. Show that

$$\frac{1+\sqrt{5}}{2} = [1, 1, 1, 1, \ldots].$$

l) Show that

$$\sqrt{1+a^2} = [a, 2a, 2a, 2a, \ldots].$$

m) Show that a *periodic* continued fraction (one where $a_{k+l} = a_k$ for some l and all large k) represents a quadratic irrational (the root of a quadratic equation with integer coefficients).

n) (*Lagrange*) Show that a quadratic irrational has a periodic continued fraction. Thus with m) this characterizes quadratic irrationals.
Hint: Suppose $r\alpha^2 + s\alpha + t = 0$ and $\alpha = [a_0, a_1, a_2, \ldots]$. Then by d),

$$\alpha = \frac{p_{n-1}\alpha'_n + p_{n-2}}{q_{n-1}\alpha'_n + q_{n-2}}.$$

Substitute this into the quadratic equation for α to obtain integers A_n, B_n, and C_n with

$$A_n(\alpha'_n)^2 + B_n\alpha'_n + C_n = 0. \tag{11.3.52}$$

Express A_n, B_n, and C_n in terms of r, s, and t and show that $A_n \neq 0$. Show that

$$B_n^2 - 4A_nC_n = s^2 - 4rt$$

and that

$$C_n = A_{n-1}.$$

Show, using f), that

$$|A_n| \le 2|r\alpha| + |r| + |s|$$
$$|C_n| \le 2|r\alpha| + |r| + |s|$$

and

$$|B_n|^2 \le 4|A_nC_n| + |s^2 - 4rt|.$$

Hence $|A_n|$, $|B_n|$, and $|C_n|$ are bounded independently of n. Thus $(A_{n_1}, B_{n_1}, C_{n_1}) = (A_{n_2}, B_{n_2}, C_{n_2}) = (A_{n_3}, B_{n_3}, C_{n_3})$ for three distinct indices n_1, n_2, and n_3, and by (11.3.52) one of

$$\alpha'_{n_1} = \alpha'_{n_2} \qquad \text{or} \qquad \alpha'_{n_1} = \alpha'_{n_3} \qquad \text{or} \qquad \alpha'_{n_2} = \alpha'_{n_3}$$

which implies the periodicity of α.

o) Show, using i), that any integral solution of Pell's equation

$$n^2 - dm^2 = 1 \qquad d \text{ a positive integer}$$

has n/m a convergent of the continued fraction of $\sqrt{d}$.

This outline of the basic theory follows Hardy and Wright [60].

3. Suppose there exists a sequence of rationals $\{p_n/q_n\}$ and $\delta > 0$ so that

$$\left|\alpha - \frac{p_n}{q_n}\right| < \frac{1}{q_n^{1+\delta}} \tag{11.3.53}$$

and

$$q_n < q_{n+1} < q_n^{1+o(1)}. \tag{11.3.54}$$

Then either

$$\frac{p}{q} = \frac{p_n}{q_n} \qquad \text{for some } n$$

or for $\varepsilon > 0$ and for $q > c_\varepsilon$

$$\left|\alpha - \frac{p}{q}\right| > \frac{1}{q^{1+1/\delta+\varepsilon}}.$$

Hint: Let $|\alpha - p/q| = 1/q^{1+1/\delta+\varepsilon'}$, $\varepsilon' > 0$, and choose n so that $\frac{1}{2}q_{n+1}^{\delta} \le q < \frac{1}{2}q_n^{\delta}$. Then

$$\left|\frac{p}{q} - \frac{p_n}{q_n}\right| < \frac{1}{q_n^{1+\delta}} + \frac{1}{q^{1+1/\delta+\varepsilon'}}$$

and if $p/q \ne p_n/q_n$,

$$1 < \frac{q}{q_n^{\delta}} + \frac{q_n}{q^{1/\delta+\varepsilon'}}.$$

The right-hand side, however, is less than 1 for q large.

4. Refine Exercise 3 to deduce Corollary 11.1, with $v := 1$, directly from Theorem 11.1.

5. (*Irrationality measure for* $e^{1/v}$) Let v be a positive integer. As in Exercise 10 of section 10.1, let

$$s_n := v^n \sum_{k=0}^{n} \frac{(2n-k)!}{(n-k)!k!} \left(\frac{1}{v}\right)^k$$

and

$$t_n := v^n \sum_{k=0}^{n} \frac{(2n-k)!}{(n-k)!k!} \left(-\frac{1}{v}\right)^k.$$

a) Show that

$$\left|e^{1/v} - \frac{s_n}{t_n}\right| = \frac{n!n!}{(2n+1)!(2n)!} e^{1/v} \left(\frac{1}{v}\right)^{2n+1} [1 + o(1)]$$

and that

$$t_n = v^n \frac{(2n)!}{n!} e^{-1/2v}[1 + o(1)].$$

Hence

$$\left|e^{1/v} - \frac{s_n}{t_n}\right| = \frac{1}{2v} \frac{\log\log t_n}{t_n^2 \log t_n} [1 + o(1)].$$

b) As in Exercises 3 and 4, show that if $p/q \ne s_n/t_n$ for some n then

$$\left|e^{1/v} - \frac{p}{q}\right| > \frac{c_v}{q^2}$$

for large q, where c_v is a positive constant depending only on v.

c) Deduce Corollary 11.1.

6. Let $d_n := \mathrm{LCM}(1, \ldots, n)$.

a) Show that there is a constant C so that

$$d_n \le C^n.$$

Hint:

$$(\Gamma_{2n} := \prod p_i) \left| \frac{(2n)!}{n!n!} \quad \text{and} \quad \frac{(2n)!}{n!n!} \le 4^n \right.$$

where the product is taken over the primes p_i, $n < p_i \le 2n$. Thus

$$d_{2n} \le \Gamma_{2n} d_n d_{\lfloor \sqrt{2n} \rfloor} \le 8^n d_n .$$

b) Let $\pi(n)$ denote the number of primes less than or equal to n. The prime number theorem asserts that

$$\pi(n) \sim \frac{n}{\log n} .$$

(See, for example, Hardy and Wright [60].) Use this to prove that

$$d_n = O(e^{\delta n}) \qquad \text{for any } \delta > 1.$$

Hint:

$$d_n = \prod p_i^{\alpha_i} \le n^{\pi(n)}$$

where the product is taken over the primes $\le n$ and where α_i is the largest integer so that $p_i^{\alpha_i} \le n$.

7. a) Show that

$$\sum_{k=1}^{K} \frac{a_1 a_2 \cdots a_{k-1}}{(x+a_1)\cdots(x+a_k)} = \frac{1}{x} - \frac{a_1 a_2 \cdots a_K}{x(x+a_1)\cdots(x+a_K)} .$$

b) Show that

$$\sum_{k=1}^{n-1} \frac{(-1)^{k-1}[(k-1)!]^2}{(n^2-1^2)\cdots(n^2-k^2)} = \frac{1}{n^2} - \frac{2(-1)^{n-1}}{n^2\binom{2n}{n}} .$$

Hint: Use a) with $x := n^2$ and $a_k := -k^2$.

c) Set

$$\delta_{n,k} := \frac{1}{2}\,\frac{(k!)^2(n-k)!}{k^3(n+k)!} .$$

Show that

$$(-1)^k n(\delta_{n,k} - \delta_{n-1,k}) = \frac{(-1)^{k-1}[(k-1)!]^2}{(n^2-1^2)\cdots(n^2-k^2)}$$

and

$$\sum_{n=1}^{N}\sum_{k=1}^{n-1} (-1)^k(\delta_{n,k} - \delta_{n-1,k}) = \sum_{n=1}^{N} \frac{1}{n^3} - 2\sum_{n=1}^{N} \frac{(-1)^{n-1}}{n^3\binom{2n}{n}}$$

$$= \sum_{k=1}^{N} (-1)^k(\delta_{N,k} - \delta_{k,k})$$

$$= \sum_{k=1}^{N} \frac{(-1)^k}{2k^3\binom{N+k}{k}\binom{N}{k}} + \frac{1}{2}\sum_{k=1}^{N} \frac{(-1)^{k-1}}{k^3\binom{2k}{k}} .$$

d) Let $N \to \infty$ in c) to deduce that

$$\zeta(3) = \frac{5}{2}\sum_{n=1}^{\infty} \frac{(-1)^{n-1}}{n^3\binom{2n}{n}} .$$

(This exercise follows van der Poorten [79] and is essentially due to Apéry.)

8. Finish the proof of Corollary 11.2.

9. (*Irrationality measures for log*)

a) Let $p_x(x) := [d/dx]^n x^n (1-x)^n$. Then as in (11.3.23),

$$p_n(x) = \sum_{k=0}^{n} \binom{n}{k}\binom{n+k}{n}(-1)^k x^k .$$

Estimate $p_n(-m)$. In particular show that for $m \in \mathbb{N}$ there exist $c_1 > 0$, c_2, c_3, and c_4 so that

$$c_1 n^{c_2}(\sqrt{m+1} + \sqrt{m})^{2n} < p_n(-m) < c_3 n^{c_4}(\sqrt{m+1} + \sqrt{m})^{2n} .$$

Hint: By Stirling's formula, up to a power of n

$$\binom{n}{k}\binom{n+k}{n} m^k \quad \text{behaves like} \quad \left[\frac{m^\alpha(1+\alpha)^{1+\alpha}}{(1-\alpha)^{1-\alpha}}\,\frac{1}{\alpha^{2\alpha}}\right]^n$$

where $k := \alpha n$. It is now a calculus exercise to maximize the above by differentiating with respect to α. The maximum occurs at $\alpha := \sqrt{m/(m+1)}$.

b) Prove that for large q,

$$\left|\log 2 - \frac{p}{q}\right| > \frac{1}{q^{4.63}} . \tag{11.3.55}$$

Outline: Let p_n be as in (11.3.22) and let

$$(11.3.36)\quad I_n := \int_0^1 \frac{p_n(x)}{1+x}\,dx = \int_0^1 \frac{p_n(x)-p_n(-1)}{1+x}\,dx + \int_0^1 \frac{p_n(-1)}{1+x}\,dx = \frac{\alpha_n}{d_n} + p_n(-1)\log 2$$

where α_n is an integer and d_n is as in Exercise 6. (Note that $(1+x)\,|\,[p_n(x)-p_n(-1)]$.) Furthermore, integrating I_n by parts n times with respect to x yields

$$(11.3.57)\qquad |I_n| = \int_0^1 \frac{x^n(1-x)^n}{(1+x)^{n+1}}\,dx\,.$$

Estimate $|I|$ from above and below by computing that the maximum of $x(1-x)/(1+x)$ occurs at $x := \sqrt{2}-1$. For large n,

$$(11.3.58)\qquad (\sqrt{2}-1-)^{2n} \le |I_n| \le (\sqrt{2}-1+)^{2n}\,.$$

From (11.3.56), (11.3.58), and part a) prove (11.3.55).

c) Prove, for $\varepsilon > 0$ and $n > N_\varepsilon$, that

$$\left|\log\frac{n+1}{n} - \frac{p}{q}\right| > \frac{1}{q^{2+\varepsilon}} \qquad q \text{ large}\,.$$

Compare (11.3.4) and (11.3.5).
Hint: Consider

$$I_n := \int_0^1 \frac{p_n(x)-p_n(-m)}{1+x/m}\,dx + \int_0^1 \frac{p_n(-m)}{1+x/m}\,dx$$

and proceed as in b). Note that

$$|I_n| = \frac{1}{m^n}\int_0^1 \frac{x^n(1-x)^n}{(1+x/m)^{n+1}}\,dx \le \frac{1}{m^n}\,\frac{1}{4^n}\,.$$

10. a) Show that $\theta_3(q)$ and $\theta_4(q)$ are irrational for rational $q := 1/n$, $n = 1, 2, 3, \ldots$.

b) (*Euler*) Show that $m^4 + n^4 = p^2$ with m, n, p integral implies $mn = 0$.

c) Use b) to show that θ_2, θ_3, and θ_4 are never all nonzero and rational.

11. a) Show that

$$(11.3.59)\qquad \left[\sum_{-\infty}^{\infty} \frac{(-1)^n}{2n+1}\right]^2 = \sum_{-\infty}^{\infty} \frac{1}{(2k+1)^2}\,.$$

Outline: Let

$$\delta_N := \sum_{-N}^{N}\sum_{-N}^{N} \frac{(-1)^{m+n}}{(2m+1)(2n+1)} - \sum_{-N}^{N} \frac{1}{(2k+1)^2}$$

and

$$\varepsilon_N := \sum_{m=-N}^{N}{}' \frac{(-1)^m}{m-n}\,.$$

Show that

$$\delta_N = \sum_{-N}^{N}\sum_{-N}^{N}{}' \frac{(-1)^{m+n}}{(2n+1)(m-n)}$$

and that

$$|\varepsilon_N| \le \frac{1}{N-n+1}\,.$$

Thus prove (11.3.59) by showing that $\delta_N \to 0$.

b) Evaluate $\zeta(2) = \pi^2/6$ from a) and Gregory's formula.

12. a) Show that for $0 \le x \le 1$, one has the following functional equation for the *dilogarithm* $\Sigma_{n=1}^{\infty} x^n/n^2$:

$$(11.3.60)\quad \log(1-x)\log x + \sum_{n=1}^{\infty} \frac{x^n}{n^2} + \sum_{n=1}^{\infty} \frac{(1-x)^n}{n^2} = \frac{\pi^2}{6}\,.$$

Hint: Show by taking derivatives that the left-hand side is zero. Evaluate the constant by letting $x \to 0$.

b) (*Euler*) Show that

$$\frac{\pi^2}{12} - \frac{1}{2}(\log 2)^2 = \sum_{n=1}^{\infty} \frac{1}{2^n n^2}\,.$$

c) Let $\mathrm{Li}_3(x)$ denote the *trilogarithm* $\Sigma_{n=1}^{\infty} x^n/n^3$. Show that, for $0 < x < 1$, the following identity due to Landen holds:

$$\mathrm{Li}_3(x) + \mathrm{Li}_3(1-x) + \mathrm{Li}_3\left(\frac{-x}{1-x}\right) - \mathrm{Li}_3(1) = \frac{\pi^2}{6}\log(1-x) - \frac{1}{2}\log(x)\log^2(1-x) + \frac{1}{6}\log^3(1-x)\,.$$

d) Deduce that $\mathrm{Li}_3(1) = \zeta(3)$ and that

i) $$\mathrm{Li}_3\left(\frac{1}{2}\right) = \frac{7}{8}\,\mathrm{Li}_3(1) - \frac{\pi^2}{12}\log 2 + \frac{1}{6}\log^3(2)$$

ii) $$\mathrm{Li}_3\left(\frac{3-\sqrt{5}}{2}\right) = \frac{4}{5}\,\mathrm{Li}_3(1) + \frac{\pi^2}{15}\log\left(\frac{3-\sqrt{5}}{2}\right) - \frac{1}{12}\log^3\left(\frac{3-\sqrt{5}}{2}\right).$$

e) Show that

$$\zeta(3) = \mathrm{Li}_3(1) = 10\int_0^{\log[(\sqrt{5}+1)/2]} t^2 \coth(t)\,dt$$

and combine this with Exercise 17a) of Section 5.5 to provide another verification of Exercise 7d). This is discussed in Lewin [81, Sec. 6.3].

13. (*Euler*) Establish

a) $$\pi[\cot(\pi x) - \cot(\pi a)] = \sum_{-\infty}^{\infty} \frac{a-x}{(x-n)(a-n)}$$

b) $$\pi^3[\cot(\pi x)\operatorname{cosec}^2(\pi x)] = \sum_{-\infty}^{\infty} \frac{1}{(x-n)^3}$$

c) $$\pi^4\left[\operatorname{cosec}^4(\pi x) - \frac{2}{3}\operatorname{cosec}^2(\pi x)\right] = \sum_{-\infty}^{\infty} \frac{1}{(x-n)^4}$$

d) $$\sum_{n=1}^{\infty} \frac{1}{4n^2-1} = \frac{1}{2}$$

e) $$\sum_{n=1}^{\infty} \frac{1}{(4n^2-1)^2} = \frac{\pi^2-8}{16}$$

f) $$\sum_{n=1}^{\infty} \frac{1}{(4n^2-1)^3} = \frac{32-3\pi^2}{64}$$

g) $$\sum_{n=1}^{\infty} \frac{1}{(4n^2-1)^4} = \frac{\pi^4+30\pi^2-384}{768}.$$

Hint: Use $x := \frac{1}{2}$ and

$$\frac{1}{2n-1} - \frac{1}{2n+1} = \frac{2}{4n^2-1}.$$

14. (*Evaluation of* $\zeta(2m)$) Define $\{B_n\}$, the *Bernoulli numbers*, by

(11.3.61) $$\frac{z}{e^z-1} + \frac{z}{2} = \sum_{m=0}^{\infty} B_{2m}\frac{z^{2m}}{(2m)!} \qquad |z| \le 2\pi$$

$B_1 := -\frac{1}{2}$ and $B_{2n+1} := 0$, $n = 1, 2, 3, \ldots$.

a) Show that

$$\sum_{k=0}^{n} \binom{n+1}{k} B_k = 0.$$

b) Show, from (11.3.61), that

$$\pi z \cot(\pi z) = \frac{2\pi i z}{e^{2\pi i z}-1} + \pi i z = \sum_{m=0}^{\infty} (-1)^m (2\pi)^{2m} \frac{B_{2m} z^{2m}}{(2m)!}$$

and from the product expansion for sin that

$$\pi\cot(\pi z) = \frac{1}{z} - \sum_{n=1}^{\infty} \frac{2z}{n^2 - z^2}.$$

c) Show that

$$\zeta(2m) := \sum_{n=1}^{\infty} \frac{1}{n^{2m}} = (-1)^{m-1}\frac{B_{2m}(2\pi)^{2m}}{2(2m)!}.$$

d) Thus

$$\zeta(2) = \frac{\pi^2}{6} \qquad \zeta(4) = \frac{\pi^4}{90} \qquad \zeta(6) = \frac{\pi^6}{945}.$$

15. (*Evaluation of* $\beta(2m+1)$) Define $\{E_{2n}\}$, *the Euler numbers*, by

(11.3.62) $$\frac{1}{\cos z} = \sum_{n=0}^{\infty} \frac{(-1)^n E_{2n} z^{2n}}{(2n)!} \qquad |z| < \frac{\pi}{2}.$$

a) Show that $E_0 = 1$ and

$$\sum_{k=0}^{n} \binom{2n}{2k} E_{2n-2k} = 0.$$

b) Show that

$$\frac{\pi}{\cos(\pi z)} = \sum_{k=0}^{\infty} 4^{k+1}\beta(2k+1)z^{2k}$$

where, as before,

$$\beta(2k+1) := \sum_{n=0}^{\infty} \frac{(-1)^n}{(2n+1)^{2k+1}} .$$

c) Show that

$$\beta(2k+1) = \frac{|E_{2k}|}{2(2k)!}\left(\frac{\pi}{2}\right)^{2k+1} .$$

d) Thus

$$\beta(1) = \frac{\pi}{4} \qquad \beta(3) = \frac{\pi^3}{32} \qquad \beta(5) = \frac{5\pi^5}{1536} .$$

There are similar evaluations for more general L functions.

16. (*Series involving* $\binom{2n}{n}$)

a) Show that

$$\frac{2x \arcsin x}{\sqrt{1-x^2}} = \sum_{m=1}^{\infty} \frac{(2x)^{2m}}{m\binom{2m}{m}} .$$

Hint: Let $f := (\arcsin x)/\sqrt{1-x^2}$. Show that

$$(1-x^2)\dot{f} = 1 + xf .$$

Show that

$$\frac{1}{2x}\sum_{m=1}^{\infty} \frac{(2x)^{2m}}{m\binom{2m}{m}}$$

also satisfies the above differential equation. (Compare Exercise 16 of Section 5.5.)

b) Show that

$$2(\arcsin x)^2 = \sum_{m=1}^{\infty} \frac{(2x)^{2m}}{m^2\binom{2m}{m}} .$$

Hint: Use a) and the fact that

$$x\,\frac{d}{dx}(\arcsin x)^2 = \frac{2x \arcsin x}{\sqrt{1-x^2}} .$$

c) Show, by differentiating in a), that

$$\sum_{m=1}^{\infty} \frac{(2x)^{2m}}{\binom{2m}{m}} = \frac{x^2}{1-x^2} + \frac{x \arcsin x}{(1-x^2)^{3/2}} .$$

d) Specialize the above series or the derivatives of the above series to show that

$$\sum_{m=1}^{\infty} \frac{1}{\binom{2m}{m}} = \frac{2\pi\sqrt{3}+9}{27}$$

$$\sum_{m=1}^{\infty} \frac{1}{m\binom{2m}{m}} = \frac{\pi\sqrt{3}}{9}$$

$$\sum_{m=1}^{\infty} \frac{1}{m^2\binom{2m}{m}} = \frac{\pi^2}{18}$$

$$\sum_{m=1}^{\infty} \frac{m}{\binom{2m}{m}} = \frac{2}{27}(\pi\sqrt{3}+9)$$

$$\sum_{m=1}^{\infty} \frac{m2^m}{\binom{2m}{m}} = \pi + 3$$

$$\sum_{m=1}^{\infty} \frac{3^m}{m^2\binom{2m}{m}} = \frac{2\pi^2}{9}$$

$$\sum_{m=1}^{\infty} \frac{3^m}{\binom{2m}{m}} = \frac{4\pi}{\sqrt{3}} + 3$$

$$\sum_{m=1}^{\infty} \frac{(-1)^{m-1}}{\binom{2m}{m}} = \frac{1}{5} + \frac{4\sqrt{5}}{25}\log\frac{\sqrt{5}+1}{2}$$

$$\sum_{m=1}^{\infty} \frac{(-1)^{m-1}}{m\binom{2m}{m}} = \frac{2}{\sqrt{5}} \log\left(\frac{\sqrt{5}+1}{2}\right)$$

$$\sum_{m=1}^{\infty} \frac{(-1)^{m}}{m^2\binom{2m}{m}} = 2\left[\log\left(\frac{\sqrt{5}+1}{2}\right)\right]^2.$$

e) Show that

$$\frac{1}{\sqrt{1-4x}} = \sum_{n=0}^{\infty} \binom{2n}{n} x^n$$

and that

$$2\log\left(\frac{1-\sqrt{1-4x}}{2x}\right) = \sum_{n=1}^{\infty} \frac{1}{n}\binom{2n}{n} x^n.$$

Thus

$$\log 4 = \sum_{n=1}^{\infty} \frac{1}{n}\left(\frac{1\cdot 3\cdots 2n-1}{2\cdot 4\cdots 2n}\right).$$

f) From e) deduce that

$$\sum_{n=1}^{\infty} \frac{\binom{2n}{n}}{2n+1} x^{2n} = \frac{1}{2x}(\arcsin 2x)$$

and that

$$\sum_{n=1}^{\infty} \frac{\binom{2n}{n}}{(2n+1)16^n} = \frac{\pi}{3}.$$

Further material is available in Lewin [81], Lehmer [85], and Zucker [85]. There is an interesting evaluation of Comtet's, namely,

$$\sum_{m=1}^{\infty} \frac{1}{m^4\binom{2m}{m}} = \frac{17\pi^4}{3240}.$$

g) We conclude with Ramanujan's

$$\sum_{m=0}^{\infty} \frac{1}{(2m+1)^2\binom{2m}{m}} = \frac{8}{3}G - \frac{\pi}{3}\log(2+\sqrt{3})$$

with G denoting Catalan's constant.
Hint: Use part a), and parts b) and h) of Exercise 10 in Section 5.6.

Bibliography

[1881] N. H. Abel, *Oeuvres Complètes* (Grondahl and Son, Christiania, 1881).

[64] M. Abramowitz and I. Stegun, *Handbook of Mathematical Functions* (Dover, New York, 1964).

[66] W. W. Adams, "Asymptotic Diophantine Approximation to *e*," *Proc. Natl. Acad. Sci.* **55** (1966), 28–31.

[66] L. V. Ahlfors, *Complex Analysis*, 2nd ed. (McGraw-Hill, New York, 1966).

[74] A. V. Aho, J. E. Hopcroft, and J. D. Ullman, *The Design and Analysis of Computer Algorithms* (Addison-Wesley, Reading, MA, 1974).

[79] K. Alladi and M. L. Robinson, "On Certain Irrational Values of the Logarithm," *Lecture Notes in Mathematics* **751**, (Springer, Berlin, 1966).

[Pr] G. Almkvist, "A Solution to a Tantalizing Problem," (in press).

[Pr] —— and B. C. Berndt, "Gauss, Landen, Ramanujan, the Arithmetic-Geometric Mean, Ellipses, the Ladies Diary, π, and the American Revolution," *MAA Monthly* (in press).

[76] G. E. Andrews, *The Theory of Partitions* (Addison-Wesley, Reading, MA, 1976).

[79] ——, "An Introduction to Ramanujan's 'Lost' Notebook," *MAA Monthly* **86** (1979), 89–108.

[86] ——, "The Fifth and Seventh Order Mock Theta Functions," *Trans. AMS* **273** (1986), 113–134.

[74] T. M. Apostol, *Mathematical Analysis*, 2d ed. (Addison-Wesley, Reading, MA, 1974).

[76*a*] ——, *Introduction to Analytic Number Theory* (Springer, New York, 1976).

[76*b*] ——, *Modular Functions and Dirichlet Series in Number Theory* (Springer, New York, 1976).

[Pr] J. Arazy, J. Claesson, S. Janson, and J. Peetre, "Means and Their Iterations."

[80] R. Askey, "Ramanujan's Extensions of the Gamma and Beta Functions," *MAA Monthly* **87** (1980), 346–359.

[81] R. Backstrom, "On Reciprocal Series Related to Fibonacci Numbers," *Fibonacci Quart.* **19** (1981), 14–21.

[Pr] D. H. Bailey, "The Computation of π to 29,360,000 Decimal Digits Using Borweins' Quartically Convergent Algorithm" (in press).

[35] W. N. Bailey, *Generalized Hypergeometric Series* (Cambridge Univ. Press, London, 1935).

[64] A. Baker, "Approximation to the Logarithms of Certain Rational Numbers," *Acta Arith.* **10** (1964), 315–323.

[75] ——, *Transcendental Number Theory* (Cambridge Univ. Press, London, 1975).

[81] G. A. Baker and P. Graves-Morris, *Padé Approximants*, vols. I and II (Addison-Wesley, Reading, MA, 1981).

[39] J. P. Ballantine, "The Best (?) Formula for Computing π to a Thousand Places," *MAA Monthly* **46** (1939), 499–501.

[50] E. F. Beckenbach, "A Class of Mean Value Functions," *MAA Monthly* **52** (1950), 1–6.

[61] —— and R. Bellman, *An Introduction to Inequalities* (Random House, New York, 1961).

[77] P. Beckmann, *A History of Pi*, 4th ed. (Golem Press, Boulder, CO, 1977).

[72] M. Beeler, R. W. Gosper, and R. Schroeppel, "Hakmem," MIT Artificial Intelligence Lab., MIT, Cambridge, MA, 1972.

[27] E. T. Bell, "Algebraic Arithmetic," *AMS Colloq*. **7**, 1927.

[61] R. Bellman, *A Brief Introduction to Theta Functions* (Holt, Rinehart and Winston, New York, 1961).

[Pr] B. C. Berndt, *The Jacobian Elliptic Functions*, Chapter 18 of Ramanujan's Second Notebook (Springer, to be published).

[Pr] B. C. Berndt, *Modular Equations of Degrees* 3, 5, *and* 7 *and Associated Theta Function Identities*, Chapter 19 of Ramanujan's Second Notebook (Springer, to be published).

[79] F. Beukers, "A Note on the Irrationality of $\zeta(2)$ and $\zeta(3)$," *Bull. London Math. Soc.* **11** (1979), 268–272.

[84] S. Bhargava and Chandrashekar Adiga, "On Some Continued Fraction Identities of Srinivasa Ramanujan," *Proc. AMS* **92** (1984), 13–18.

[Pr] A. J. Biagioli, "A Proof of Two Identities of Ramanujan."

[73] G. Birkhoff, *A Source Book in Classical Analysis* (Harvard Univ. Press, Cambridge, MA, 1973).

[69] —— and G. C. Rota, *Ordinary Differential Equations*, 2d ed. (Blaisdell, Waltham, MA, 1969).

[1888] C. W. Borchardt, *Gesammelte Werke* (Berlin, 1888).

[66] A. Borel, S. Chowla, C. S. Herz, K. Iwasawa, and J. P. Serre, "Seminar on Complex Multiplication," *Lecture Notes in Mathematics* **21** (Springer, Berlin, 1966).

[75] A. Borodin and I. Munro, *The Computational Complexity of Algebraic and Numeric Problems* (American Elsevier, New York, 1975).

[86] D. Borwein and J. M. Borwein, "Alternating Series in Several Dimensions," *MAA Monthly* (1986) to appear.

[85] ——, ——, and K. F. Taylor, "Convergence of Lattice Sums and Madelung's Constant," *J. Math. Phys.* **26** (1985), 2299–3009.

[85] J. M. Borwein, "Some Modular Identities of Ramanujan Useful in Approximating π," *Proc. AMS* **95** (1985), 365–371.

[83] —— and P. B. Borwein, "A Very Rapidly Convergent Product Expansion for π," BIT **23** (1983), 538–540.

[84*a*] —— and ——, "The Arithmetic-Geometric Mean and Fast Computation of Elementary Functions," *SIAM Rev.* **26** (1984), 351–365.

[84*b*] —— and ——, "Cubic and Higher Order Algorithms for π," *Can. Math. Bull.* **27** (1984), 436–443.

[84*c*] —— and ——, "Explicit Algebraic *N*th Order Approximations to Pi," in *Approximation Theory and Spline Functions*, NATO ASI Ser., S. P. Singh, J. H. W. Burry, and B. Watson, Eds. (Reidel, Dordrecht, 1984).

[84*d*] ——, "Reduced Complexity Calculation of Log," Dalhousie Technical Report.

[86] —— and ——, "More Quadratically Converging Algorithms for π," *Math Comput.* **46** (1986), 247–253.

[Pr] J. M. Borwein and P. B. Borwein, "Approximating π with Ramanujan's Solvable Modular Equations" (in press).

[85] P. B. Borwein, "On the Complexity of Computing Factorials," *J. Algorithms* **6** (1985), 376–380.

[Pr] ——, "Problem," *SIAM Rev.* (in press).

[53] F. Bowman, *Introduction to Elliptic Functions* (English Universities Press, London, 1953).

[68] C. B. Boyer, *A History of Mathematics* (Wiley, New York, 1968).

[84] D. Braess, "On the Conjecture of Meinardus on Rational Approximation to e^x, II," *J. Approx. Theory* **40** (1984), 375–379.

[76*a*] R. P. Brent, "Fast Multiple-Precision Evaluation of Elementary Functions," *J. ACM* **23** (1976), 242–251.

[76*b*] ——, "Multiple-Precision Zero-Finding Methods and the Complexity of Elementary Function Evaluation," in *Analytic Computational Complexity*, J. F. Traub, Ed. (Academic Press, New York, 1976).

[76*c*] ——, "The Complexity of Multiple-Precision Arithmetic," in *Complexity of Computational Problem Solving*, R. S. Anderssen and R. P. Brent, Eds. (Univ. of Queensland Press, Brisbane, 1976).

[80] —— and G. M. MacMillan, "Some New Algorithms for High-Precision Calculation of Euler's Constant," *Math. Computat.* **34** (1980), 305–312.

[83] D. M. Bressoud, "An Easy Proof of the Rogers–Ramanujan Identities," *J. Number Theory* **16** (1983), 235–241.

[1875] C. Briot and J. C. Bouquet, *Théorie des Fonctions Elliptiques* (Paris, 1875).

[26] T. J. I. A. Bromwich, *An Introduction to the Theory of Infinite Series*, 2d ed. (Macmillan, London, 1926).

[71] P. Bundschuh, "Irrationalitätsmasse für e^a, $a \neq 0$ rational oder Liouville-Zahl," *Math. Ann.* **192** (1971), 229–242.

[84] V. I. Buslaev, A. A. Gonchar, and S. P. Suetin, "On the Convergence of Subsequences of the *n*th Row of a Padé Table," *Math. U.S.S.R. Sbornik* **48** (1984), 535–540.

[71] L. Carlitz, "Reduction Formulae for Fibonacci Summations," *Fibonacci Quart.* **9** (1971), 449–466, 510.

[71] B. C. Carlson, "Algorithms Involving Arithmetic and Geometric Means," *MAA Monthly* **78** (1971), 496–505.

[72] ——, "The Logarithmic Mean," *MAA Monthly* **79** (1972), 615–618.

[75] ——, "Invariance of an Integral Average of a Logarithm," *MAA Monthly* **82** (1975), 379–382.

[77] ——, *Special Functions of Applied Mathematics* (Academic Press, New York, 1977).

[78] ——, "Short Proofs of Three Theorems on Elliptic Integrals," *SIAM J. Math. Anal.* **9** (1978), 524–528.

[57] J. W. S. Cassels, *An Introduction to Diophantine Approximation* (Cambridge Univ. Press, London, 1957).

[1874] A. Cayley, "A Memoir on the Transformations of Elliptic Functions," *Phil. Trans.* **164** (1874), 397–456.

[1895] ——, *An Elementary Treatise on Elliptic Functions* (Bell and Sons, 1895; republished Dover, New York, 1961).

[85] K. Chandrasekharan, *Elliptic Functions* (Springer, Berlin, 1985).

[66] E. W. Cheney, *Introduction to Approximation Theory* (McGraw-Hill, New York, 1966).

[84] D. V. Chudnovsky and G. V. Chudnovsky, "Padé and Rational Approximation to Systems of Functions and Their Arithmetic Applications," *Lecture Notes in Mathematics* **1052** (Springer, Berlin, 1984).

[71] A. Clark, *Elements of Abstract Algebra* (Wadsworth, Belmont, CA, 1971).

[Pr] J. E. Cohen and R. D. Nussbaum, "Arithmetic-Geometric Means of Positive Matrices" (in press).

[69] S. A. Cook and S. O. Aanderaa, "On the Minimum Computation of Functions," *Trans. AMS* **142** (1969), 291–314.

[65] J. W. Cooley and J. W. Tukey, "An Algorithm for the Machine Calculation of Complex Fourier Series," *Math. Comp.* **19** (1965), 297–301.

[67] ——, P. A. Lewis, and P. D. Welch, "History of the Fast Fourier Transform," *Proc. IEEE* **55** (1967), 1675–1677.

[84] D. A. Cox, "The Arithmetic-Geometric Mean of Gauss," *L'Enseignement Math.* **30** (1984), 275–330.

[85] ——, "Gauss and the Arithmetic-Geometric Mean," *Notices of the AMS* **32** (1985), 147–151.

[81] J. H. Davenport, "On the Integration of Algebraic Functions," *Lecture Notes in Computer Science* **102** (Springer, Berlin, 1981).

[79] C. S. Davis, "A Note on Rational Approximation," *Bull. Austral. Math. Soc.* **20** (1979), 407–410.

[84] C. Denninger, "On the Analogue of the Formula of Chowla and Selberg for Real Quadratic Fields," *J. Reine Ang. Math.* **351** (1984), 171–191.

[29] L. E. Dickson, *Introduction to the Theory of Numbers* (Dover, New York, 1929).

[71] ——, *History of the Theory of Numbers*, vols. I–III (1919, 1920, 1923), reprinted Chelsea, New York, 1971).

[65] M. Dutta and L. Debnath, *Elements of the Theory of Elliptic and Associated Functions* (World Press Private, Calcutta, 1965).

[73] P. Du Val, *Elliptic Functions and Elliptic Curves* (Cambridge Univ. Press, London, 1973).

[58] A. Eagle, *The Elliptic Functions as They Should Be* (Galloway and Porter, Cambridge, 1958).

[79] C. H. Edwards, Jr., *The Historical Development of the Calculus* (Springer, New York, 1979).

[53] A. Erdélyi et al., *Higher Transcendental Functions*, vols. 1–3 (McGraw-Hill, New York, 1953–1955).

[81] J. A. Ewell, "An Easy Proof of the Triple-Product Identity," *MAA Monthly* **88** (1981), 270–272.

[82] ——, "Consequences of Watson's Quintuple Product Identity," *Fibonacci Quart.* **20** (1982), 256–262.

[83] ——, "A Simple Proof of Fermat's Two-Square Theorem," *MAA Monthly* **90** (1983), 635–637.

[86] J. A. Ewell, "On the enumerator for sums of three squares," *Fibonacci Quart.* **24** (1986), 151–153.

[84*a*] D. M. E. Foster and G. M. Phillips, "The Arithmetic-Harmonic Mean," *Math. Comput.* **42** (1984), 183–191.

[84*b*] —— and ——, "A Generalization of the Archimedean Double Sequence," *J. Math. Anal. Appl.* **101** (1984), 575–581.

[1866] C. F. Gauss, *Werke* (Göttingen, 1866–1933), vol. 3, pp. 361–403.

[38] C. Gini, "Di una Formula Compressiva delle Medie," *Metron.* **13** (1938), 3–22.

[80] M. L. Glasser and I. J. Zucker, "Lattice Sums in Theoretical Chemistry," *Advances and Perspectives* **5** (1980), 67–139.

[85] D. Goldfeld, "Gauss' Class Number Problem for Imaginary Quadratic Fields," *Bull. AMS* **13** (1985), 23–37.

[61] B. Gordon, "Some Identities in Combinatorial Analysis," *Quart. J. Math.* **12** (1961), 285–290.

[84] H. W. Gould and M. E. Mays, "Series Expansions of Means," *J. Math. Anal. Appl.* **101** (1984), 611–621.

[1881] E. M. Goursat, "Sur l'Équation Différentielle Linéaire qui Admet pour Intégrale la Série Hypergéométrique," *Ann. Sci. l'Ecole Normale Sup.* (2) **10** (1881), 3–142.

[80] I. S. Gradshteyn and I. M. Ryzhik, *Table of Integrals, Series and Products* (Academic Press, New York, 1980).

[1892] A. G. Greenhill, *The Applications of Elliptic Functions* (1892; republished Dover, New York, 1959).

[09] H. Hancock, *Theory of Elliptic Functions* (1909, republished Dover, New York, 1958).

[28] M. Hannah, "The Modular Equations," *Proc. London Math. Soc.* **28** (1928), 46–52.

[75] E. R. Hansen, *A Table of Series and Products* (Prentice-Hall, Englewood Cliffs, NJ, 1975).

[40] G. H. Hardy, *Ramanujan* (Cambridge Univ. Press, London, 1940).

[59] ——, J. E. Littlewood, and G. Polya, *Inequalities*, 2d ed. (Cambridge Univ. Press, London, 1959).

[60] —— and E. M. Wright, *An Introduction to the Theory of Numbers*, 4th ed. (Oxford Univ. Press, London, 1960).

[77] P. Henrici, *Applied and Computational Complex Analysis*, vols. 1 and 2 (Wiley, New York, 1974, 1977).

[12] C. Hermite, *Oeuvres*, vol. 3 (Paris, 1912), pp. 150–181.

[17] ——, *Oeuvres*, vol. 4 (Paris, 1917), pp. 357–377.

[05] —— and T. J. Stieltjes, *Correspondence d'Hermite et de Stieltjes*, vol. 2 (Gauthiers-Villars, Paris, 1905).

[1893] D. Hilbert, *Math. Ann.* **43** (1893), 216–219.

[85] M. D. Hirschhorn, "A Simple Proof of Jacobi's Two Square Theorem," *MAA Monthly* **92** (1985), 579–580.

[70] A. S. Householder, *The Numerical Treatment of a Single Nonlinear Equation* (McGraw-Hill, New York, 1970).

[82] L. K. Hua, *Introduction to Number Theory* (Springer, Berlin, 1982).

[84] D. Hughes, Master's Thesis, Dalhousie Univ., Halifax, NS, 1984.

[1796] J. Ivory, "A New Series for the Rectification of the Ellipsis; Together with Some Observations on the Evolution of the Formula $(a^2 + b^2 - 2ab(\cos\phi)^n)$," *Trans. Roy. Soc. Edinburgh* **4** (1796), 177–190.

[1829] G. J. Jacobi, "Fundamenta Nova Theoriae Functionum Ellipticorum," 1829; *Jacobi's Gesammelte Werke*, vol. 1 (Berlin, 1881–1891), pp. 49–239.

[84] E. Kaltofen and N. Yui, "On the Modular Equation of Order 11," *Proc. 1984 MACSYMA User's Conf.*, pp. 472–485.

[Pr] Y. Kanada, Y. Tamura, S. Yoshino, and Y. Ushiro, "Calculations of π to 10,013,395 Decimal Places Based on Gauss–Legendre Algorithm and Gauss Arctangent Relation," preprint (1983).

[57] I. Kaplansky, *An Introduction to Differential Algebra* (Hermann, Paris, 1957).

[86] M. Keith, "Circle digits a self-referential story," *The Mathematical Intelligencer* **8** (1986), 56–57.

[64] A. Khinchin, *Continued Fractions* (Chicago Univ. Press, Chicago, 1964).

[24] L. V. King, *On the Direct Numerical Calculation of Elliptic Functions and Integrals* (Cambridge Univ. Press, London, 1924).

[1897] F. Klein, *Famous Problems of Elementary Geometry*, transl. by W. Beman and D. E. Smith (Ginn and Co., Boston, 1897).

[79] ——, "Development of Mathematics in the 19th Century," 1928, *Trans., Math. Sci. Press*, R. Hermann Ed. (Brookline, MA, 1979).

[1892] —— and R. Fricke, *Vorlesungen über die Theorie der Elliptischen Modulfunktionen* (Teubner, Leipzig, 1890, 1892).

[81] D. Knuth, *The Art of Computer Programming*, vol. 2: *Seminumerical Algorithms* 2nd ed. (Addison-Wesley, Reading, MA 1981).

[71] A. Krazer, *Lehrbuch der Theta-Funktionen* (Chelsea, New York, 1971).

[78] H. T. Kung and J. F. Traub, "All Algebraic Functions Can be Computed Fast," *J. ACM* **25** (1978), 245–260.

[1899] E. Landau, "Sur la Série des Invers de Nombres de Fibonacci," *Bull. Soc. Math. France* **27** (1899), 298–300.

[58] E. Landau, *Elementary Number Theory* (Chelsea, New York, 1958).

[66*a*] S. Lang, *Introduction to Transcendental Numbers* (Addison-Wesley, Reading MA, 1966).

[66*b*] ——, *Introduction to Diophantine Approximation* (Addison-Wesley, Reading, MA 1966).

[73] ——, *Elliptic Functions* (Addison-Wesley, Reading, MA, 1973).

[78] E. B. Leach and M. C. Sholander, "Extended Mean Values," *MAA Monthly* **85** (1978), 84–90.

[1811] A. M. Legendre, *Exercises de Calcul Intégral*, vols. 1–3 (Paris, 1811–1819).

[38] D. H. Lehmer, "On Arctangent Relations for π," *MAA Monthly* **45** (1938), 657–664.

[71] ——, "On the Compounding of Certain Means," *J. Math. Anal. Appl.* **36** (1971), 183–200.

[85] ——, "Interesting Series Involving the Central Binomial Coefficient," *MAA Monthly* **92** (1985), 449–457.

[66] J. Lehner, *A Short Course in Automorphic Functions* (Holt, Rinehart and Winston, New York, 1966).

[80] *Le Petit Archimède*, no. 64–65, "Numéro Spécial π" (1980).

[77] W. J. LeVeque, *Fundamentals of Number Theory* (Addison-Wesley, Reading, MA, 1977).

[81] L. Lewin, *Polylogarithms and Associated Functions* (North Holland, New York, 1981).

[74] Tung-Po Lin, "The Power Mean and the Logarithmic Mean,' *MAA Monthly* **81** (1974), 879–883.

[1882] F. Lindemann, "Über die Zahl π," *Math. Ann.* **20** (1882), 213–225.

[1884] J. Liouville, "Sur des Classes Trés Étendues de Quantités dont la Valeur n'est ni Rationnelle ni même Réductible à des Irrationnelles Algébriques," *Compt. Rend.* **18** (1844), 883–885, 910–911.

[81] J. D. Lipson, *Elements of Algebra and Algebraic Computing* (Addison-Wesley, Reading, MA, 1981).

[66] W. Magnus, *Formulas and Theorems for the Special Functions of Mathematical Physics* (Springer, Berlin, 1966).

[31] K. Mahler, "Zur Approximations der Exponentialfunktion und des Logarithmus, I, II," *J. Reine Ang. Math.* **166** (1931), 118–136, 137–150.

[53] ——, "On the Approximation of π," *Indagiones Math.* **15** (1953), 30–42.

[67] ——, "Application of Some Formulae by Hermite to the Approximation of Exponentials and Logarithms," *Math. Ann.* **168** (1967), 200–227.

[75] D. Masser, "Elliptic Functions and Transcendence," *Lecture Notes in Mathematics* **437** (Springer, Berlin, 1975).

[83] G. Miel, "On Calculations Past and Present: The Archimedean Algorithm," *MAA Monthly* **90** (1983), 17–35.

[74] M. Mignotte, "Approximations Rationalles de π et Quelques Autres Nombres," *Bull. Soc. Math. France*, Mem. **37** (1974), 121–132.

[70] D. S. Mitrinovic, *Analytic Inequalities* (Springer, New York, 1970).

[16] L. J. Mordell, "Note on Class Relation Formulae," *Messenger of Math.* **45** (1916), 75–80.

[77] G. Nemeth, "Relative Rational Approximation of the Function e^x," *Math. Notes* **21** (1977), 325–328.

[69] R. Nevanlinna and V. Paatero, *Introduction to Complex Analysis* (Addison-Wesley, Reading, MA, 1969).

[79] D. J. Newman, "Approximation with Rational Functions," *AMS Regional Conf. Ser. in Mathematics*, no. 41 (1979).

[82] ——, "Rational Approximation Versus Fast Computer Methods," *Lectures on Approximation and Value Distribution* (Presses de l'Université de Montréal, Montreal, 1982), pp. 149–174.

[85] ——, "A Simplified Version of the Fast Algorithms of Brent and Salamin," *Math. Comput.* **44** (1985), 207–210.

[84] M. Newman and D. Shanks, "On a Sequence Arising in Series for π," *Math. Comput.* **42** (1984), 191–217.

[56] I. Niven, "Irrational Numbers," *Carus Math. Monograph* **11** (MAA, 1956).

[78] M. Nyvoll, 'Tilnoermelsesformler for Ellipsebuer," *BIT* **25–26** (1978), 70–72.

[80] J. Oxtoby, *Measure and Category*, 2d ed. (Springer, New York, 1980).

[81] G. M. Phillips, "Archimedes the Numerical Analyst," *MAA Monthly* **88** (1981), 165–169.

[84] ——, "Archimedes and the Complex Plane," *MAA Monthly* **91** (1984), 108–114.

[73] H. Rademacher, *Topics in Analytic Number Theory* (Springer, Berlin, 1973).

[60] E. D. Rainville, *Special Functions* (Macmillan, New York, 1960).

[84] K. G. Ramanathan, "On Ramanujan's Continued Fraction," *Acta Arith.* **43** (1984), 209–225.

[14] S. Ramanujan, "Modular Equations and Approximations to π," *Quart. J. Math.* **45** (1914), 350–372.

[62] ——, *Collected Papers* (Chelsea, New York, 1962).

[77] R. Rankin, *Modular Forms and Functions* (Cambridge Univ. Press, London, 1977).

[73] H. E. Rauch and A. Lebowitz, *Elliptic Functions, Theta Functions and Riemann Surfaces* (Williams and Wilkins, Baltimore, MD, 1973).

[84] P. Ribenboim, "Consecutive Powers," *Expo. Math.* **2** (1984), 193–221.

[85] ——, "Representation of Real Numbers by Means of Fibonacci Numbers," *L'Enseignement Mathematiques* **3** (1985), 249–259.

[27] J. F. Ritt, "Meromorphic Functions with Addition or Multiplication Theorems," *Trans. AMS* **29** (1927), 341–360.

[48] ——, *Integration in Finite Terms* (Columbia Univ. Press, New York, 1948).

[72] M. Rosenlicht, "Integration in Finite Terms," *MAA Monthly* **79** (1972), 963–972.

[76] E. Salamin, "Computation of π Using Arithmetic-Geometric Mean," *Math. Comput.* **30** (1976), 565–570.

[82] T. Sasaki and Y. Kanada, "Practically Fast Multiple-Precision Evaluation of log (x)," *J. Inf. Process.* **5** (1982), 247–250.

[50] H. C. Schepler, "The Chronology of Pi," *Math. Mag.* (1950), 165–170, 216–228, 279–283.

[77] I. J. Schoenberg, "On the Arithmetic-Geometric Mean," *Delta* **7** (1977), 49–65.

[82] ——, *Mathematical Time Exposures* (MAA, Washington, DC, 1982).

[76] B. Schoenberg, *Elliptic Modular Functions* (Springer, Berlin, 1976).

[71] A. Schönhage and V. Strassen, "Schnelle Multiplikation Grosser Zahlen," *Computing* **7** (1971), 281–292.

[67] A. Selberg and S. Chowla, "On Epstein's Zeta-Function." *J. Reine Ang. Math.* **227** (1967), 86–110.

[82] D. Shanks, "Dihedral Quartic Approximations and Series for π," *J. Number Theory* **14** (1982), 397–423.

[62] —— and J. W. Wrench, Jr., "Calculation of π to 100,000 Decimals," *Math. Comput.* **16** (1962), 76–99.

[1853] W. Shanks, *Contributions to Mathematics Comprising Chiefly of the Rectification of the Circle to 607 Places of Decimals* (G. Bell, London, 1853).

[85] D. Singmaster, "The Legal Values of Pi," *Math. Intelligencer* **7** (1985), 67–72.

[66] L. J. Slater, *Generalized Hypergeometric Functions* (Cambridge Univ. Press, London, 1966).

[85] E. U. Stickel, "Fast Computation of Matrix Exponential and Logarithms," *Analysis* **5** (1985), 163–173.

[74] K. B. Stolarsky, *Algebraic Numbers and Diophantine Approximation* (Marcel Dekker, New York, 1974).

[75] ——, "Generalizations of the Logarithmic Mean," *Math. Mag.* **48** (1975), 87–92.

[80] ——, "The Power and Generalized Logarithmic Means," *MAA Monthly* **87** (1980), 545–548.

[63] D. Sweeney, "On the Computation of Euler's Constant," *Math. Comput.* **17** (1963), 170–178.

[Pr] Y. Tamura and Y. Kanada, "Calculation of π to 4,196,393 Decimals Based on Gauss–Legendre Algorithm," *Math Comput.* (in press).

[1893] J. Tannery and J. Molk, *Fonctions Elliptiques*, vols. 1 and 2 (1893; republished Chelsea, New York, 1972).

[49] J. Todd, "A Problem on Arctangent Relations," *MAA Monthly* **8** (1949), 517–528.

[75] ——, "The Leminiscate Constants," *Communication of the ACM* **18** (1975), 14–19.

[79] ——, *Basic Numerical Mathematics*, vol. 1 (Academic Press, New York, 1979).

[84] L. Trefethen, "The Asymptotic Accuracy of Rational Best Approximations to e^z on a Disk," *J. Approx. Theory* **40** (1984), 380–383.

[65] F. G. Tricomi, "Sull 'Algoritmo Iterativo del Borchardt e su di una sua Generalizzazione," *Rend. Arc. Mat. Palermo* **14** (1965), 85–94.

[79] A. van der Poorten, "A Proof that Euler Missed. . . , Apéry's Proof of the Irrationality of $\zeta(3)$," *Math. Intelligencer* **1** (1979), 195–203.

[85] S. Wagon, "Is π Normal," *The Mathematical Intelligencer* **7** (1985), 65–67.

[74] M. Waldschmidt, "Nombres Transcendants," *Lecture Notes in Mathematics* **402** (Springer, New York, 1974).

[69] J. L. Walsh, "Interpolation and Approximation by Rational Functions in the Complex Domain," *AMS Colloq. Publ.* **20**, 5th ed. (1969).

[Pr] G. Walz, "Effiziente Berechnung spezieller Funktionen mittels asymptotischer Entwicklungen und Eliminationsprozeduren (Mannheim).

[29] G. N. Watson, "Theorems Stated by Ramanujan (VII): Theorems on Continued Fractions," *J. London Math. Soc.* **4** (1929), 39–48.

[32] ——, "Some Singular Moduli (1)," *Quart. J. Math.* **3** (1932), 81–98.

[33] ——, "The Marquis and the Land Agent," *Math. Gaz.* **17** (1933), 5–17.

[35] ——, "Generating Functions of Class Numbers," *Compos. Math.* **1** (1935), 39–68.

[08] H. Weber, *Lehrbuch der Algebra* (1908 republished Chelsea, New York, 1980).

[67] K. Weierstrass, *Werke*, vol. 2 (republished Frankfurt, 1967), pp. 341–362.

[76] A. Weil, *Elliptic Functions According to Eisenstein and Kronecker* (Springer, New York, 1976).

[27] E. T. Whittaker and G.N. Watson, *A Course of Modern Analysis*, 4th ed. (Cambridge Univ. Press, London, 1927).

[84] J. Wimp, *Computation with Recurrence Relations* (Pitman, London, 1984).

[80] S. Winograd, "Arithmetic Complexity of Computations," *SIAM Reg. Conf. Ser. in Applied Mathematics* **33** (1980).

[60] J. W. Wrench, Jr., "The Evolution of Extended Decimal Approximations to π," *Math. Teacher* **53** (1960), 644–650.

[77] I. J. Zucker, "The Evaluation in Terms of Γ-Functions of the Periods of Elliptic Curves Admitting Complex Multiplication," *Math. Proc. Cambridge Phil. Soc.* **82** (1977), 111–118.

[79] ——, "The Summation of Series of Hyperbolic Functions," *SIAM J. Math. Anal.* **10** (1979), 192–206.

[84] ——, "Some Infinite Series of Exponential and Hyperbolic Functions," *SIAM J. Math. Anal.* **15** (1984), 406–413.

[85] ——, "On the Series $\Sigma_{k=1}^{\infty} \binom{2k}{k}^{-1} k^{-n}$ and Related Sums," *J. Number Theory* **20** (1985), 92–102.

[76*a*] —— and M. M. Robertson, "Some Properties of Dirichlet L-Series," *J. Phys. A* **9** (1976), 1207–1214.

[76*b*] —— and ——, A Systematic Approach to the Evaluation of $\Sigma_{(m,n\neq 0,0)}(am^2+bmn+cn^2)^{-s}$," *J. Phys. A* **9** (1976), 1215–1225.

Symbol List

Symbol	Description	Section	Formula
AGM	Arithmetic-Geometric Mean Iteration	1.1	1.1.1 and 1.1.2
$M(\cdot,\cdot)$	Common limit of the AGM	1.1	1.1.5
$AG(\cdot,\cdot)$	Common limit of the AGM	1.1	
a_n, b_n, c_n	Variables in the AGM	1.1	
k_n	Legendre form of the AGM	1.1	1.1.11
k'	$k' := \sqrt{1-k^2}$, Complementary modulus	1.1	
$\dot{f}$	the derivative of f	1.1	
$K(k)$	$K(k) := \int_0^{\pi/2} \frac{d\theta}{\sqrt{1-k^2\sin^2\theta}} = \int_0^1 \frac{dt}{\sqrt{(1-t^2)(1-k^2t^2)}}$ complete elliptic integral of the 1st kind	1.3	1.3.1
$E(k)$	$E(k) := \int_0^{\pi/2} \sqrt{1-k^2\sin^2\theta}\, d\theta = \int_0^1 \frac{\sqrt{1-k^2t^2}}{\sqrt{1-t^2}}\, dt$ complete elliptic integral of the 2nd kind	1.3	1.3.2
$K'(k)$	$K'(k) := K(k')$	1.3	1.3.3
$E'(k)$	$E'(k) := E(k')$	1.3	1.3.4
$F(a, b; c, z)$	Hypergeometric function	1.3	1.3.5
$(2i-1)!!$	$(2i-1)!! := 1\cdot 3\cdot 5\cdot \ldots \cdot(2i-1)$	1.3	
$I(\cdot,\cdot)$	$I(a,b) := \int_0^{\pi/2} \frac{d\theta}{\sqrt{a^2\cos^2\theta + b^2\sin^2\theta}} = \frac{1}{a} K'\left(\frac{b}{a}\right)$	1.4	1.4.4
$J(\cdot,\cdot)$	$J(a,b) := \int_0^{\pi/2} \sqrt{a^2\cos^2\theta + b^2\sin^2\theta}\, d\theta = aE'\left(\frac{b}{a}\right)$	1.4	1.4.5
G	$G(k) := k^{1/2}k'K(k)$	1.5	
G^*	$G^*(k) = k^{1/2}k'K'(k)$	1.5	
Γ	$\Gamma(x) := \int_0^\infty e^{-t}t^{x-1}\, dt$, Gamma function	1.6	1.6.4

Symbol	Description	Section	Formula
β	$\beta(x,y) := \int_0^1 t^{x-1}(1-t)^{y-1}\, dt$, Beta function	1.6	1.6.5
$sn(u,k)$	$u := \int_0^{sn(u,k)} \frac{dt}{\sqrt{(1-t^2)(1-k^2t^2)}}$	1.7 2.7	1.7.1 2.7.5
$cn(u,k)$	$u := \int_1^{cn(n,k)} \frac{dt}{\sqrt{(1-t^2)(k'^2+k^2t^2)}}$	1.7 2.7	1.7.2 2.7.6
$dn(u,k)$	$u := \int_1^{dn(u,k)} \frac{dt}{\sqrt{(1-t^2)(t^2-k'^2)}}$	1.7 2.7	1.7.3 2.7.7
p	$p(z) := \frac{1}{z^2} + \sum_{w\in L'} \left(\frac{1}{(z-w)^2} - \frac{1}{w^2}\right)$ Weierstrass function	1.7	
θ_2	$\theta_2(q) := \sum_{n=-\infty}^{\infty} q^{(n+1/2)^2}$	2.1	2.1.1
θ_3	$\theta_3(q) := \sum_{n=-\infty}^{\infty} q^{n^2}$	2.1	2.1.2
θ_4	$\theta_4(q) := \sum_{n=-\infty}^{\infty} (-1)^n q^{n^2}$	2.1	2.1.3
r_2	$r_2(n) :=$ number of representations of n as a sum of two squares	2.2	
$\theta_i(s)$	$\theta_i(s) := \theta_i(q)$ where $q := e^{-\pi s}$	2.2	
$k(q)$	$k(q) := k = \theta_2^2(q)/\theta_3^2(q)$	2.3	
$k'(q)$	$k'(q) := k' = \theta_4^2(q)/\theta_3^2(q)$	2.3	
$K(k)$	$K(k) = \frac{\pi}{2}\theta_3^2(q)$	2.3	
q	$q = e^{-K'(k)/K(k)}$	2.3	
$k(s)$	$k(s) := k(q)$ where $q := e^{-\pi s}$	2.3	
$\theta_i(z,q)$	General theta functions	2.6	2.6.1
$\theta_j(q)$	Theta functions in q, $z := 0$	2.6	
$\theta_j(z)$	Theta functions in z, q suppressed	2.6	
$\theta(z)$	Theta functions in z, q and j suppressed	2.6	
Q_0	$Q_0(q) := \prod_{n=1}^{\infty} (1-q^{2n})$	3.1	3.1.3
Q_1	$Q_1(q) := \prod_{n=1}^{\infty} (1+q^{2n})$	3.1	3.1.3
Q_2	$Q_2(q) := \prod_{n=1}^{\infty} (1+q^{2n-1})$	3.1	3.1.3
Q_3	$Q_3(q) := \prod_{n=1}^{\infty} (1-q^{2n-1})$	3.1	3.1.3
λ^*	$\lambda^*(r) := k(q)$ where $q = e^{-\pi\sqrt{r}}$	3.2	
θ_1^+	$\theta_1^+(q) := 2\sum_{n=0}^{\infty} (-1)^n(2n+1)q^{(n+1/2)^2}$	3.2	

Symbol	Description	Section	Formula
θ_5	$\theta_5(q) := 2\sum_{n=-\infty}^{\infty}(-1)^n q^{(2n-1/2)^2}$	3.2	3.2.5
θ_6^+	$\theta_6^+(q) := 2\sum_{n=0}^{\infty}(-1)^{n(n-1)/2}(2n+1)q^{(n+1/2)^2}$	3.2	3.2.6
η	$q^{1/12}Q_0$, Eta function	3.2	3.2.9
f	$q^{-1/24}Q_3$	3.2	3.2.9
f_1	$\sqrt{2}q^{1/12}Q_1$	3.2	3.2.9
f_2	$q^{-1/24}Q_2$	3.2	3.2.9
Σ'	$\sum_{n,m=-\infty}^{\infty}{}' a_{m,n} := \sum_{\substack{n,m=-\infty \\ a_{m,n}\neq\infty}} a_{m,n}$	3.2	
G_n	$G_n := (2kk')^{-1/12} = 2^{-1/4}f(\sqrt{-n})$	3.2	3.2.13
g_n	$g_n := \left(\frac{k'^2}{2k}\right)^{1/12} = 2^{-1/4}f_1(\sqrt{-n})$	3.2	3.2.13
$\binom{n}{m}_q$	Gaussian or q-binomial coefficients	3.3	3.3.1
$(q)_s$	$(q)_s := \prod_{m=1}^{\infty}(1-q^m)/(1-q^{s+m})$	3.3	3.3.2
r_4	$r_4(n) :=$ number of representations of n as a sum of four squares	3.5	3.5.1
σ_1	$\sigma_1(n) := \sum_{d \mid n} d$	3.5	
$w(n)$	$w(n) := \sigma_1(n) + \sigma_1(\text{odd}\,(n))$	3.5	3.5.2
$S(p, q)$	$S(p,q) := \sum_{r=0}^{q-1} e^{-\pi i r^2 p/q}$	3.5	
$M(f)$	$M(f) := M_s(f) := \int_0^\infty f(x)x^{s-1}dx$, Mellin transform	3.6	3.6.1
ζ	$\zeta(s) := \sum_{n=1}^{\infty} n^{-s}$, Riemann zeta function	3.6	
$g(t)$	$g(t) := (\theta_3(t)-1)/2$	3.6	
$L(\beta)$	$L(\beta) := \sum_{n=1}^{\infty}\frac{\beta^n}{1-\beta^n}$, $\lvert\beta\rvert < 1$, Lambert series	3.7	3.7.5
F_n	$F_0 := 0,\ F_1 := 1,\ F_{n+1} := F_n + F_{n-1}$, Fibonacci numbers	3.7 (Ex. 3)	
L_n	$L_0 := 2,\ L_1 := 1,\ L_{n+1} := L_n + L_{n-1}$, Lucas numbers	3.7	
$\mathcal{H}$	$\mathcal{H} := \{\text{im}(\tau) > 0\}$	4.3	
$\mathcal{H}^*$	$\mathcal{H}^* := \mathcal{H} \cup \{i\infty\} \cup \{\mathbb{Q}\}$	4.3	
Γ-group	Inhomogeneous modular group	4.3	
λ-group		4.3	
F_Γ	Fundamental set of Γ-group	4.3	
F_λ	Fundamental set of λ-group	4.3	

Symbol	Description	Section	Formula
S_Γ	$\begin{pmatrix}1&1\\0&1\end{pmatrix}$	4.3 (Ex. 1)	
T_Γ	$\begin{pmatrix}0&-1\\1&0\end{pmatrix}$	4.3 (Ex. 1)	
S_λ	$\begin{pmatrix}1&2\\0&1\end{pmatrix}$	4.3 (Ex. 1)	
T_λ	$\begin{pmatrix}1&0\\2&1\end{pmatrix}$	4.3 (Ex. 1)	
λ	$\lambda(t) := k^2(t) = \left[\frac{\theta_2(q)}{\theta_3(q)}\right]^4$, $q := e^{i\pi t}$	4.3	
J	$J(t) := \frac{4}{27}\frac{(1-\lambda(t)+\lambda^2(t))^3}{\lambda^2(t)(1-\lambda(t))^2}$, Klein's absolute invariant	4.3	
j	$j(t) := 1728J(t)$	4.3	
T_p	$\left\{\begin{pmatrix}a&b\\c&d\end{pmatrix}: ad-bc=p;\ a,b,c,d \in \mathbb{Z}\right\}$ transformations of order p	4.4	4.4.1
A_p	$A_p := \begin{pmatrix}p&0\\0&1\end{pmatrix}$	4.4	
A_i	$A_i := \begin{pmatrix}1&i\\0&p\end{pmatrix}$, $i = 0, 1, \ldots, p-1$	4.4	
B_p	$B_p := \begin{pmatrix}p&0\\0&1\end{pmatrix}$	4.4	
B_i	$B_i := \begin{pmatrix}1&2i\\0&p\end{pmatrix}$, $i = 0, 1, \ldots, p-1$	4.4	
W_p	$W_p(x,\lambda) := \prod_{i=0}^{p}(x-\lambda_i)$, $\lambda_i := \lambda \circ B_i$ pth order modular equation for λ	4.4	4.4.2
F_p	$F_p(x,j) = \prod_{i=0}^{p}(x-j_i)$, $j_i := j \circ A_i$ pth order modular equation for j	4.4	4.4.6
$\mathbb{Q}_p$	$\mathbb{Q}$ adjoin the pth roots of unity	4.4	
Ω_p	$\Omega_p(v,u) := \prod_{i=0}^{p}(v-u_i)$ pth order modular equation for u	4.5	4.5.1
u_p	$u_p := (-1)^{(p^2-1)/8}(\lambda(q^p))^{1/8} := (t-1)^{(p^2-1)/8}u(q^p)$, $q = e^{i\pi t}$	4.5	4.5.1
u_k	$u_k := (\lambda(\alpha^{8k}q^{1/p}))^{1/8} := u(\alpha^{8k}q^{1/p})$, $k = 0, 1, \ldots, p-1$, $\alpha = e^{2i\pi/p}$	4.5	4.5.1
M_p	$M_p(l,k) := \frac{\theta_3^2(q)}{\theta_3^2(q^{1/p})} = \frac{K(k)}{K(l)}$, Multiplier of order p	4.6	4.6.1
k_p	$k_p := k(e^{-\pi\sqrt{p}})$ pth singular value	4.6	
l_p	$l_p := k_p' = k(e^{-\pi/\sqrt{p}})$	4.6	
$\alpha(r)$	$\alpha(r) := \frac{E'}{K} - \frac{\pi}{4K^2}$, $k := k(e^{-\pi\sqrt{r}})$	5.1	5.1.1

Symbol	Description	Section	Formula
$\delta(r)$	$\delta(r) := \sqrt{r} - 2\alpha(r)$	5.1	5.1.9
R_p	$R_p(l, k) := \dfrac{pP(q) - P(q^{1/p})}{\theta_3^2(q)\theta_3^2(q^{1/p})}$	5.2	5.2.7
P	$P(q) := 1 - 24 \sum_{n=1}^{\infty} \dfrac{nq^{2n}}{1 - q^{2n}}$	5.2	5.2.8
ε_p	$\varepsilon_p(l, k) := \dfrac{pkk'^2}{M_p(l, k)} \cdot \dfrac{dM_p}{dk}(l, k) + M_p^{-2}(l, k)l^2 - pk^2$	5.2	5.2.11
σ	$\sigma(p) := R_p(k', k)$, $k := e^{-\pi\sqrt{p}}$	5.2	5.2.12
k_n	For $n \in \mathbb{N}$, compute k_{n+1} by solving $W_p(k_n^2, k_{n+1}^2) = 0$	5.4	
m_n	$m_n := M_p^{-1}(k_n, k_{n+1})$	5.4	5.4.1
r_n	$r_n := R_p(k_n, k_{n+1})$	5.4	5.4.1
ε_n	$\varepsilon_n := [m_n r_n + m_n^2(1 + k_n^2) - p(1 + k_{n+1}^2)]/3$	5.4	5.4.1
α_{n+1}	$\alpha_{n+1} := m_n^2 \alpha_n - p^n \sqrt{r} \varepsilon_n$	5.4	5.4.2
${}_2F_1$	${}_2F_1(a, b; c; x) := \sum_{n=0}^{\infty} \dfrac{(a)_n (b)_n}{(c)_n} \dfrac{x^n}{n!}$, where	5.5	5.5.1
$(a)_n$	$(a)_n := \dfrac{\Gamma(a+n)}{\Gamma(a)} = a(a+1)\ldots(a+n-1)$, rising factorial	5.5	
${}_3F_2$	${}_3F_2(a, b, c; d, e; x) := \sum_{n=0}^{\infty} \dfrac{(a)_n (b)_n (c)_n}{(d)_n (e)_n} \dfrac{x^n}{n!}$	5.5	5.5.2
K_s	$K_s(k) := \dfrac{\pi}{2} \cdot {}_2F_1\left(\dfrac{1}{2} - s, \dfrac{1}{2} + s; 1; k^2\right)$	5.5	5.5.3
E_s	$E_s(k) := \dfrac{\pi}{2} \cdot {}_2F_1\left(-\dfrac{1}{2} - s, \dfrac{1}{2} + s; 1; k^2\right)$	5.5	5.5.4
G	$G := \sum_{n=0}^{\infty}{}' \dfrac{1}{(2n+1)^2}$, Catalan's constant	5.6 (Ex. 10)	
$\Omega(a_n)$	$b_n = \Omega(a_n)$ if $b_n = O(a_n)$ and $a_n = O(b_n)$	6.1	
O_B	Bit complexity	6.1	
O_{op}	Operational complexity	6.1	
FFT	Fast Fourier Transform	6.2	
$M(n)$	Bit complexity of multiplication	6.4 6.3 (Ex. 3)	
$D(n)$	Bit complexity of division	6.4	
$R(n)$	Bit complexity of root extraction	6.4	
$a \wedge b$	$a \wedge b := \min(a, b)$	8.1	8.1.1
$a \vee b$	$a \vee b : \max(a, b)$	8.1	8.1.1
t_M	$t_M(x) := M(x, 1)$, M a mean, the trace	8.1	
$\mathbb{R}^{\times}$	$\mathbb{R} - \{0\}$	8.1	
M_f	$M_f(a, b) := f^{-1}M(f(a), f(b))$	8.1	
M_p	M_p denotes M_f when $f(x) = x^p$	8.1	

Symbol	Description	Section	Formula
H_p	$H_p(a, b) := \left(\dfrac{a^p + b^p}{2}\right)^{1/p}$, $a, b > 0$, Hölder means	8.1	8.1.7
${}_pM$	${}_pM(a, b) := \dfrac{M(a^p, b^p)}{M(a^{p-1}, b^{p-1})} = \dfrac{M_p^p(a, b)}{M_{p-1}^{p-1}(a, b)}$	8.1	8.1.9
L_p	$L_p(a, b) = \dfrac{a^p + b^p}{a^{p-1} + b^{p-1}}$, Lehmer means	8.1	8.1.1
$G_{s,r}$	$G_{s,r}(a, b) := \left[\dfrac{a^s + b^s}{a^r + b^r}\right]^{1/s-r}$, Gini means	8.1	8.1.1
$M_{\int_f}$	$M_{\int_f}(a, b) := \left[\dfrac{\int_a^b f(x)\,dx}{b - a}\right]$, $a \neq b$	8.1	8.1.1
S_p	$S_p(a, b) := M_{\int x^{p-1}}(a, b) = \left[\dfrac{a^p - b^p}{p(a - b)}\right]^{1/p-1}$, $p \neq 0, 1$, Stolarsky means	8.1	8.1.1
$\mathscr{L}$	$\mathscr{L}(a, b) := S_0(a, b)$, Logarithmic mean	8.1	8.1.1
$\mathscr{I}$	$\mathscr{I}(a, b) := S_1(a, b)$, Identric mean	8.1	8.1.1
$E_{r,s}$	$E_{r,s}(a, b) := \left[\dfrac{s(a^r - b^r)}{r(a^s - b^s)}\right]^{1/(r-s)}$	8.1	8.1.1
$M > N$	$M(\phi(a), \phi(b)) = \phi(N(a, b))$, dominance	8.2	
$M \sim N$	if $M > \phi_1 N$ and $N > \phi_2 M$, equivalence	8.2	
$M \otimes N$	Compound Mean of M and N	8.3	8.3.1
$M \leq N$	M comparable to N	8.3	
$M \otimes_g N$	The Gaussian product (Def. 8.2)	8.3	
$[M, N]_g$	The Gaussian mean iterative process (Def. 8.2)	8.3	
$M \otimes_a N$	The Archimedean product (Def. 8.2)	8.3	
$[M, N]_a$	The Archimedean mean iterative process (Def. 8.2)	8.3	
N^*	$N^*(a, b) = N(M(a, b), b)$		
$\tilde{M}$	$\tilde{M}(a, b) := M(a \wedge b, a \vee b)$	8.3	8.3.5
$R(\alpha; \delta, \delta'; x^2, y^2)$	$R(\alpha; \delta, \delta'; x^2, y^2) := \dfrac{1}{\beta(\alpha, \alpha')} \int_0^{\infty} t^{\alpha'-1}(t + x^2)^{-\delta}(t + y^2)^{-\delta'}\,dt$	8.5	8.5.1
C_{ij}	$C_{ij} := F_i \otimes F_j$ $(i, j = 1, 2, 3, 4)$	8.5	8.5.3
F_1	$F_1(a, b) := \dfrac{a + b}{2}$	8.5	8.5.3
F_2	$F_2(a, b) := \sqrt{ab}$	8.5	8.5.3
F_3	$F_3(a, b) := \sqrt{\dfrac{a + b}{2} \cdot a}$	8.5	8.5.3
F_4	$F_4(a, b) := \sqrt{\dfrac{a + b}{2} \cdot b}$	8.5	8.5.
$\operatorname{arcsl}(x)$	$\operatorname{arcsl}(x) := \int_0^x (1 - s^4)^{-1/2}\,ds$	8.5	8.5.
$\operatorname{arcslh}(x)$	$\operatorname{arcslh}(x) := \int_0^x (1 + s^4)^{-1/2}\,ds$	8.5	8.5.

Symbol	Description	Section	Formula
$\bar{a}$	$\bar{a} := (a_1, \ldots, a_N)$	8.7	
$L_p(\bar{a})$	$L_p(\bar{a}) := \left(\sum_{i=1}^{N} a_i^p\right) \Big/ \left(\sum_{i=1}^{N} a_i^{p-1}\right)$, Lehmer means	8.7	8.7.3
$H_p(\bar{a})$	$H_p(\bar{a}) := \left(\frac{1}{N} \sum_{i=1}^{N} a_i^p\right)^{1/p}$, Hölder means	8.7	8.7.4
$\bigotimes_{i=1}^{N} M_i$	The common limit (when it exists) of $[M^1, \ldots, M^n]$	8.7	
$[M^1, \ldots, M^N]$	$a_{n+1}^i := M^i(\bar{a}_n)$, or vectorially $\bar{a}_{n+1} = \bar{M}(\bar{a}_n)$	8.7	8.7.5
$\bigotimes_{g\,i=1}^{N} M^i$	N-dimensional Gaussian product	8.7	
$\bigotimes_{a\,i=1}^{N} M^i$	N-dimensional Archimedean product	8.7	8.7.6
He(a, c)	He$(a, c) := \frac{a + \sqrt{ac} + c}{3}$, Heronian mean	8.7	8.7.8
$S(a, c)$	$S(a, c) := \text{He} \otimes_g G(a, c)$	8.7	
$M_{J_N f}$	$M_{J_N f}(a_0, a_1, \ldots, a_N) := f^{-1}\left[\sum_{k=0}^{N} \frac{N!\,F_{(N)}(a_k)}{\Pi_{k \neq j}(a_k - a_j)}\right]$	8.7	8.7.10
$TG(f\colon F)$	The algebraic transformation group of f over F	8.8	
$b_3(2s)$	$b_3(2s) := \sum_{i,j,k=-\infty}^{\infty}{}' \frac{(-1)^{i+j+k}}{(i^2 + j^2 + k^2)^s}$	9.2	9.2.1
$b_2(2s)$	$b_2(2s) := \sum_{i,j=-\infty}^{\infty}{}' \frac{(-1)^{i+j}}{(i^2 + j^2)^s}$	9.2	9.2.2
$b_4(2s)$	$b_4(2s) := \sum_{i,j,k,l=-\infty}^{\infty}{}' \frac{(-1)^{i+j+k+l}}{(i^2 + j^2 + k^2 + l^2)^s}$	9.2	9.2.3
$\alpha(s)$	$\alpha(s) := \sum_{n=1}^{\infty} \frac{(-1)^{n+1}}{n^s} = (1 - 2^{1-s})\zeta(s)$,	9.2	
$\beta(s)$	$\beta(s) := \sum_{n=0}^{\infty} \frac{(-1)^n}{(2n+1)^s}$	9.2	
$L_{\pm d}(s)$	$L_{\pm d}(s) := \sum_{n=1}^{\infty} (\pm d \mid n) n^{-s}$	9.2 (Ex. 6)	
$(a; q)_\infty$	$(a; q)_\infty := \prod_{k=0}^{\infty} (1 - aq^k)$	9.4 (Ex. 7)	9.4.5
$M_p(n)$	$M_p(k_n, k_{p^2 n})$	9.5	
N_p	$N_p := \eta^2(q)/\eta^2(q^{1/p})$, η given by 3.2.9	9.5	9.5.15
D_δ	$D_\delta := \{z \in \mathbb{C} \mid \lvert z \rvert \le \delta\}$	10.1	
P_n	Algebraic polynomials of degree n	10.1	
$\lVert f \rVert_A$	$\lVert f \rVert_A := \sup_{x \in A} \lvert f(x) \rvert$	10.1	10.1.1
$E_n(f, A)$	$E_n(f, A) := \min_{p \in P_n} \lVert f - p \rVert_A$	10.1	10.1.2

Symbol	Description	Section	Formu
$R_n(f, A)$	$R_n(f, A) := R_n(f) = \min_{p,q \in P_n} \lVert f - p/q \rVert_A$	10.1	10.1.
γ	$\gamma := \lim_{m \to \infty}\left[1 + \frac{1}{2} + \frac{1}{3} + \cdots + \frac{1}{m} - \log m\right]$, Euler's constant	10.2	10.2.
d_n	$d_n := \text{LCM}(1, 2, \ldots, n)$	11.3	
$[a_0, a_1, \ldots, a_n]$	$[a_0, a_1, \ldots, a_n] := a_0 + \cfrac{1}{a_1 + \cfrac{1}{a_2 + \ddots + a_2 + \cfrac{1}{a_n}}}$ simple continued fraction	11.3 (Ex. 2)	
$[a_0, a_1, \ldots]$	$\lim_{n \to \infty} [a_0, a_1, \ldots, a_n]$	11.3 (Ex. 2)	
B_n	$\frac{z}{e^z - 1} + \frac{z}{2} = \sum_{m=0}^{\infty} B_{2m} \frac{z^{2m}}{(2m)!}$, $\lvert z \rvert \le 2\pi$; $B_1 = -\frac{1}{2}$ and $B_{2n+1} := 0$, $n = 1, 2, 3,$ Bernoulli numbers	11.3	11.3.
E_{2n}	$\frac{1}{\cos z} = \sum_{n=0}^{\infty} \frac{(-1)^n E_{2n} z^{2n}}{(2n)!}$, $\lvert z \rvert < \frac{\pi}{2}$, Euler numbers	11.3	11.3

Author Index

Numbers in parenthesis indicate references in the Bibliography. "Pr" indicates references in press.

Subject Index