APPENDIX II: INTEGER RELATIONS

The USES of LLL and PSLQ

▶ A vector $(x_1, x_2, \cdots, x_n)$ of reals *possesses an integer relation* if there are integers a_i not all zero with

$$\boxed{0 = a_1 x_1 + a_2 x_2 + \cdots + a_n x_n.}$$

PROBLEM: Find a_i if such exist. If not, obtain lower bounds on the size of possible a_i.

- $(n = 2)$ *Euclid's algorithm* gives solution.

- $(n \geq 3)$ Euler, Jacobi, Poincare, Minkowski, Perron, others sought method.

- *First general algorithm* in 1977 by **Ferguson** & Forcade. Since '77: **LLL** (in Maple), HJLS, PSOS, **PSLQ** ('91, *parallel* '99).

▶ Integer Relation Detection was recently ranked among "the 10 algorithms with the greatest influence on the development and practice of science and engineering in the 20th century." J. Dongarra, F. Sullivan, *Computing in Science & Engineering* **2** (2000), 22–23.

Also: Monte Carlo, Simplex, Krylov Subspace, QR Decomposition, Quicksort, ..., FFT, Fast Multipole Method.

A. ALGEBRAIC NUMBERS

Compute α to sufficiently high precision ($O(n^2)$) and apply LLL to the vector

$$(1, \alpha, \alpha^2, \cdots, \alpha^{n-1}).$$

- Solution integers a_i are coefficients of a polynomial likely satisfied by α.

- If no relation is found, exclusion bounds are obtained.

B. FINALIZING FORMULAE

▶ If we suspect an identity PSLQ is powerful.

- (*Machin's Formula*) We try `PSLQ` on

$$[\arctan(1), \arctan(\frac{1}{5}), \arctan(\frac{1}{239})]$$

and recover `[1, -4, 1]`. That is,

$$\frac{\pi}{4} = 4\arctan(\frac{1}{5}) - \arctan(\frac{1}{239}).$$

[Used on all serious computations of π from 1706 (100 digits) to 1973 (1 million).]

- (*Dase's 'mental' Formula*) We try `PSLQ` on

$$[\arctan(1), \arctan(\frac{1}{2}), \arctan(\frac{1}{5}), \arctan(\frac{1}{8})]$$

and recover `[-1, 1, 1, 1]`. That is,

$$\frac{\pi}{4} = \arctan(\frac{1}{2}) + \arctan(\frac{1}{5}) + \arctan(\frac{1}{8}).$$

[Used by Dase for 200 digits in 1844.]

C. ZETA FUNCTIONS

▶ The *zeta function* is defined, for $s > 1$, by

$$\zeta(s) = \sum_{n=1}^{\infty} \frac{1}{n^s}.$$

• Thanks to *Apéry* (1976) it is well known that

$$S_2 := \zeta(2) = 3 \sum_{k=1}^{\infty} \frac{1}{k^2 \binom{2k}{k}}$$

$$A_3 := \zeta(3) = \frac{5}{2} \sum_{k=1}^{\infty} \frac{(-1)^{k-1}}{k^3 \binom{2k}{k}}$$

$$S_4 := \zeta(4) = \frac{36}{17} \sum_{k=1}^{\infty} \frac{1}{k^4 \binom{2k}{k}}$$

▶ These results *strongly* suggest that

$$\aleph_5 := \zeta(5) / \sum_{k=1}^{\infty} \frac{(-1)^{k-1}}{k^5 \binom{2k}{k}}$$

is a simple rational or algebraic number. Yet, **PSLQ shows**: if $\aleph_5$ satisfies a polynomial of degree ≤ 25 the Euclidean norm of coefficients *exceeds* 2×10^{37}.

D. ZAGIER'S CONJECTURE

For $r \geq 1$ and $n_1, \ldots, n_r \geq 1$, consider:

$$L(n_1, \ldots, n_r; x) := \sum_{0<m_r<\ldots<m_1} \frac{x^{m_1}}{m_1^{n_1} \ldots m_r^{n_r}}\,.$$

Thus

$$L(n; x) = \frac{x}{1^n} + \frac{x^2}{2^n} + \frac{x^3}{3^n} + \cdots$$

is the classical *polylogarithm*, while

$$\begin{aligned} L(n,m;x) &= \frac{1}{1^m}\frac{x^2}{2^n} + (\frac{1}{1^m} + \frac{1}{2^m})\frac{x^3}{3^n} + (\frac{1}{1^m} + \frac{1}{2^m} + \frac{1}{3^m})\frac{x^4}{4^n} \\ &+ \cdots, \\ L(n,m,l;x) &= \frac{1}{1^l}\frac{1}{2^m}\frac{x^3}{3^n} + (\frac{1}{1^l}\frac{1}{2^m} + \frac{1}{1^l}\frac{1}{3^m} + \frac{1}{2^l}\frac{1}{3^m})\frac{x^4}{4^n} + \cdots\,. \end{aligned}$$

- The series converge absolutely for $|x| < 1$ and conditionally on $|x| = 1$ unless $n_1 = x = 1$.

These polylogarithms

$$L(n_r, \ldots, n_1; x) = \sum_{0<m_1<\ldots<m_r} \frac{x^{m_r}}{m_r^{n_r} \ldots m_1^{n_1}},$$

are *determined uniquely* by the *differential equations*

$$\frac{d}{dx} L(\mathbf{n_r}, \ldots, n_1; x) = \frac{1}{x} L(\mathbf{n_r - 1}, \ldots, n_2, n_1; x)$$

if $n_r \geq 2$ and

$$\frac{d}{dx} L(\mathbf{n_r}, \ldots, n_2, n_1; x) = \frac{1}{1-x} L(\mathbf{n_{r-1}}, \ldots, n_1; x)$$

if $n_r = 1$ with the *initial conditions*

$$L(n_r, \ldots, n_1; 0) = 0$$

for $r \geq 1$ and

$$L(\emptyset; x) \equiv 1.$$

Set $\overline{s} := (s_1, s_2, \ldots, s_N)$. Let $\{\overline{s}\}_n$ denotes concatenation, and $w := \sum s_i$.

Then every *periodic* polylogarithm leads to a function

$$L_{\overline{s}}(x,t) := \sum_n L(\{\overline{s}\}_n; x) t^{wn}$$

which solves an algebraic ordinary differential equation in x, and leads to nice *recurrences*.

A. In the simplest case, with $N = 1$, the ODE is $\mathbf{D_s F = t^s F}$ where

$$D_s := \left((1-x)\,\frac{d}{dx}\right)^1 \left(x\,\frac{d}{dx}\right)^{s-1}$$

and the solution (by series) is a generalized hypergeometric function:

$$L_{\overline{s}}(x,t) = 1 + \sum_{n \geq 1} x^n \frac{t^s}{n^s} \prod_{k=1}^{n-1} \left(1 + \frac{t^s}{k^s}\right),$$

as follows from considering $D_s(x^n)$.

B. Similarly, for $N = 1$ and negative integers

$$L_{\overline{-s}}(x,t) := 1 + \sum_{n\geq 1} (-x)^n \frac{t^s}{n^s} \prod_{k=1}^{n-1} \left(1 + (-1)^k \frac{t^s}{k^s}\right),$$

and $L_{\overline{-1}}(2x-1,t)$ solves a hypergeometric ODE.

▶ Indeed

$$L_{\overline{-1}}(1,t) = \frac{1}{\beta(1+\frac{t}{2}, \frac{1}{2} - \frac{t}{2})}.$$

C. We may obtain ODEs for eventually periodic Euler sums. Thus, $L_{-2,1}(x,t)$ is a solution of

$$\begin{aligned}
t^6\, F &= x^2(x-1)^2(x+1)^2\, D^6 F \\
&+ x(x-1)(x+1)(15x^2-6x-7)\, D^5 F \\
&+ (x-1)(65x^3+14x^2-41x-8)\, D^4 F \\
&+ (x-1)(90x^2-11x-27)\, D^3 F \\
&+ (x-1)(31x-10)\, D^2 F + (x-1)\, DF.
\end{aligned}$$

- This leads to a four-term recursion for $F = \sum c_n(t)x^n$ with initial values $c_0 = 1, c_1 = 0, c_2 = t^3/4, c_3 = -t^3/6$, and the ODE can be simplified.

We are now ready to prove Zagier's conjecture. Let $F(a, b; c; x)$ denote the *hypergeometric function*. Then:

Theorem 2 (BBGL) *For* $|x|, |t| < 1$ *and integer* $n \geq 1$

$$\begin{aligned} \sum_{n=0}^{\infty} \quad & L(\underbrace{3, 1, 3, 1, \ldots, 3, 1}_{n-fold}; x)\, t^{4n} \\ = \quad & F\left(\frac{t(1+i)}{2}, \frac{-t(1+i)}{2}; 1; x\right) \\ \times \quad & F\left(\frac{t(1-i)}{2}, \frac{-t(1-i)}{2}; 1; x\right). \end{aligned} \tag{9}$$

Proof. Both sides of the putative identity start

$$1+\frac{t^4}{8}x^2+\frac{t^4}{18}x^3+\frac{t^8+44t^4}{1536}x^4+\cdots$$

and are *annihilated* by the differential operator

$$D_{31} := \left((1-x)\,\frac{d}{dx}\right)^2 \left(x\,\frac{d}{dx}\right)^2 - t^4\,.$$

QED

- Once discovered — and it was discovered after much computational evidence — this can be checked variously in Mathematica or Maple (e.g., in the package *gfun*)!

Corollary 3 *(***Zagier Conjecture***)*

$$\zeta(\underbrace{3,1,3,1,\ldots,3,1}_{n-fold}) = \frac{2\,\pi^{4n}}{(4n+2)!} \qquad (10)$$

Proof. We have

$$F(a,-a;1;1) = \frac{1}{\Gamma(1-a)\Gamma(1+a)} = \frac{\sin \pi a}{\pi a}$$

where the first equality comes from Gauss's evaluation of $F(a,b;c;1)$.

Hence, setting $x = 1$, in (9) produces

$$F\left(\frac{t(1+i)}{2}, \frac{-t(1+i)}{2}; 1; 1\right) F\left(\frac{t(1-i)}{2}, \frac{-t(1-i)}{2}; 1; 1\right)$$

$$= \frac{2}{\pi^2 t^2} \sin\left(\frac{1+i}{2}\pi t\right) \sin\left(\frac{1-i}{2}\pi t\right)$$

$$= \frac{\cosh \pi t - \cos \pi t}{\pi^2 t^2} = \sum_{n=0}^{\infty} \frac{2\pi^{4n} t^{4n}}{(4n+2)!}$$

on using the Taylor series of cos and cosh. Comparing coefficients in (9) ends the proof. **QED**