## Experimental Computation and Visual Theorems: The Computer as Collaborator

## Jonathan Borwein FRSC FAAS FAA FBAS

(With Aragón, Bailey, P. Borwein, Skerritt, Straub, Tam, Wan, Zudilin, ...)

Centre for Computer Assisted Research Mathematics and its Applications
The University of Newcastle, Australia

http://carma.newcastle.edu.au/meetings/evims/

## For 2015 Presentations

Revised 22-05-15

## Prepared for Wollongong



## Dedicated to Jacques Hadamard, A Universal Mathematician (1998)


> "The object of mathematical rigor is to sanction and legitimize the conquests of intuition, and there was never any other object for it."-JSH (1865-1963)
last dozen of the first hundred of his year", said at the celebration of Hadamard's centenary:


#### Abstract

The taupin who saw Jacques Hadamard enter the lecture theatre, found a teacher who was active, alive, whose reasoning combined exactness and dynamism. Thus the lecture became a struggle and an adventure. Without rigour suffering, the importance of intuition was restored to us, and the better students were delighted. For the others, the intellectual life was less comfortable, but so exciting... And then, above all, we knew quite well that with such a guide we never risked going under [II.5, p. 8].


Mandelbrojt recalled at the same jubilee:

For several years, Hadamard also gave lectures at the Collège de France: lectures which were long, hard, infinitely interesting. He never tried to hide the difficulties, on the contrary he brought them out. The audience thought together with him; these lectures provoked creativity. The day after a lecture by Hadamard was rich, full and all day long one thought about the ideas.

It was in these lectures that I learnt the secrets of the function $\zeta(s)$ of Riemann, it was there that I understood the significance of analytic continuation, of quasi-analyticity, of Dirichlet series, of the role of functional calculus in the calculus of variations [II.5, p. 25-27].

## EXTENDED ABSTRACT

Long before current graphic, visualisation and geometric tools were available, John E. Littlewood (1885-1977) wrote in his delightful Miscellany ${ }^{1}$ :

A heavy warning used to be given [by lecturers] that pictures are not rigorous; this has never had its bluff called and has permanently frightened its victims into playing for safety. Some pictures, of course, are not rigorous, but I should say most are (and I use them whenever possible myself). [p. 53]

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Over the past decade, the role of visual computing in my own research has expanded dramatically.

In part this was made possible by the increasing speed and storage capabilities-and the growing ease of programming-of modern multi-core computing environments [BMC].

[^1]But, at least as much, it has been driven by my group's paying more active attention to the possibilities for graphing, animating or simulating most mathematical research activities.

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- I first briefly discuss both visual theorems and experimental computation.
- I then turn to dynamic geometry (iterative reflection methods $[A B]$ ) and matrix completion problems (applied to protein conformation [ABT]). ${ }^{2}$ (Case studies I)

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- I then turn to dynamic geometry (iterative reflection methods $[A B]$ ) and matrix completion problems (applied to protein conformation [ABT]). ${ }^{2}$ (Case studies I)
- After an algorithmic interlude (Case studies II), I end with description of work from my group in probability (behaviour of short random walks [BS, BSWZ]) and transcendental number theory (normality of real numbers [AB3]). (Case studies III)

[^4]
## My plans



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- What we have seen and heard so far
- My inclinations on the day
- How I manage my time


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JMB was among roughly 60 new 2015 Fellows of the American Mathematical Society. He was cited "For contributions to nonsmooth analysis and classical analysis as well as experimental mathematics and visualization of mathematics."

## Key References and URLS

AB F. Aragon and J.M. Borwein,"Global convergence of a non-convex Douglas-Rachford iteration." J. Global Optim. 57(3) (2013), 753-769.
AB3 F. Aragon, D. H. Bailey, J.M. Borwein and P.B. Borwein, "Walking on real numbers." Mathematical Intelligencer. 35(1) (2013), 42-60.
ABT F. Aragon, J. M.Borwein, and M. Tam, '"Douglas-Rachford feasibility methods for matrix completion problems. ANZIAM Journal. Accepted March 2014. Available at http://arxiv.org/abs/1308.4243.
BS J.M. Borwein and A. Straub, "Mahler measures, short walks and logsine integrals." Theoretical Computer Science. Special issue on Symbolic and Numeric Computation. 479 (1) (2013), 4-21. DOI: http: / / link. springer.com/article/10.1016/j.tcs.2012.10.025.
BSC J.M. Borwein, M. Skerritt and C. Maitland, "Computation of a lower bound to Giuga's primality conjecture." Integers 13 (2013). Online Sept 2013 at \#A67,
http://www.westga.edu/~integers/cgi-bin/get.cgi.
BSWZ J.M. Borwein, A. Straub, J. Wan and W. Zudilin (with an Appendix by Don Zagier), "Densities of short uniform random walks." Can. J. Math. 64(5), (2012), 961-990.
http://dx.doi.org/10.4153/CJM-2011-079-2.


NAMS 2005. KnotPlot in a Cave

Considerable obstacles generally present themselves to the beginner, in studying the elements of Solid Geometry, from the practice which has hitherto uniformly prevailed in this country, of never submitting to the eye of the student, the figures on whose properties he is reasoning, but of drawing perspective representations of them upon a plane.

I hope that I shall never be obliged to have recourse to a perspective drawing of any figure whose parts are not in the same plane.-Augustus De Morgan

[^5]
## Contents

(1) PART I: Visual Theorems - Visual theorems

- Large matrices
- Experimental mathematics

Digital Assistance

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- Simulation in Mathematics

3
PART II. Case Studies

- la. Iterated reflections
- lb: Protein conformation
- Ila: 100 digit challenge
- Ilb: Polylogarithms

PART III: Randomness

- Randomness is slippery
- Normality
- Normality of Pi
- BBP Digit Algorithms
- Some background
- Illa. Short rambles

Number walks

- Number walks (base four)


## Walks on 'reals'

- IIIb: Study of number walks
- IIIc: Stoneham numbers
(8) Features of our walks
- Expected distance to origin
- Number of points visited
- Fractal and box-dimension


## Other realisations

- Fractals everywhere
- 3D drunkard's walks
- Chaos games
- 2-automatic numbers
- Walks on the genome
- References


## Visual Theorems:

## Animation, Simulation and Stereo ...

See http://vis.carma.newcastle.edu.au/: Stoneham movie


Cinderella, 3.14 min of Pi, Catalan's constant and Passive 3D

## Visual Theorems:

See http://vis.carma.newcastle.edu.au/: Stoneham movie
The latest developments in computer and video technology have provided a multiplicity of computational and symbolic tools that have rejuvenated mathematics and mathematics education. Two important examples of this revitalization are experimental mathematics and visual theorems
— ICMI Study 19 (2012)


Cinderella, 3.14 min of Pi, Catalan's constant and Passive 3D

## Visualising large matrices

Large matrices often have structure that pictures will reveal but which numeric data may obscure.

- The picture shows a $25 \times 25$ Hilbert matrix on the left and on the right a matrix required to have $50 \%$ sparsity and non-zero entries random in $[0,1]$.


Figure: The Hilbert matrix (L) and a sparse random matrix (R)

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## Visualising large matrices

The $4 \times 4$ Hilbert matrix is
$\left[\begin{array}{cccc}1 & 1 / 2 & 1 / 3 & 1 / 4 \\ 1 / 2 & 1 / 3 & 1 / 4 & 1 / 5 \\ 1 / 3 & 1 / 4 & 1 / 5 & 1 / 6 \\ 1 / 4 & 1 / 5 & 1 / 6 & 1 / 7\end{array}\right]$

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Hilbert matrices are notoriously unstable numerically. The left of the Figure shows the inverse of the $20 \times 20$ Hilbert matrix computed symbolically exactly. The middle shows enormous numerical errors if one uses 10 digit precision, and the right even if one uses 20 digits.


Figure: Inverse $20 \times 20$ Hilbert matrix (L) and 2 numerical inverses (R)

## Me and my collaborators



## MAA 3.14

http://www. carma.newcastle.edu.au/jon/pi-monthly.pdf

## 2012 walk on $\pi$ (went viral)

Biggest mathematics picture ever?


Figure: Walk on first 100 billion base-4 digits of $\pi$ (normal?).

## 2012 walk on $\pi$ (went viral)

Biggest mathematics picture ever?

Resolution: 372,224×290,218 pixels (108 gigapixels)

Computation: took roughly a month where several parts of the algorithm were run in parallel with 20 threads on CARMA's MacPro cluster.

Figure: Walk on first 100 billion base-4 digits of $\pi$ (normal?).
http://gigapan.org/gigapans/106803
Jonathan Borwein (University of Newcastle, Australia)
Visual Theorems

## Outreach:

## images and animations led to high-level research which went viral



## Wired UK August 2013

## Spotastape and reinvent maths

This rendering of the first 100 billion digits of pi proves they're
random - unless you see a pattern

Ihis image is a representation of the first 100 billion digits of pi. "I was interested to see what I'd get by turning a number into a picture," says mathematician Jon Borwein, from the University of Newcastle in Australia, who collaborated with programmer Fran Aragon. "We wanted to prove, with the image, that the digits of pi are really random," explains Aragon. "If they weren't, the picture would have a structure or a specifically repeating shape, like a circle, or some broccoli."

This image is equivalent to 10,000 photos from a ten-megapixel camera, and it can be explored in Gigapan. The technique doesn't only confirm established theories -it provides insights: during the drawing of a supposedly random sequence called the "Stoneham number", Aragon noticed a regularly occurring shape within the figure. "We wereable to show that the Stoneham number is not random in base 6 , $^{\prime \prime}$ he explains. "We would never have known this without visualising it." MV carma.newcastle.edu. aw/piwalk.shtml

## (D) Tap to watch the first 100 Wi-F or 3 G required

## Outreach:

images and animations led to high-level research which went viral


- 100 billion base four digits of $\pi$ on Gigapan
- Really big pictures are often better than movies (NASA and AMS)


## My number-walk collaborators



## My short-walk collaborators



James Wan


Armin Straub


Wadim Zudilin

## My short-walk collaborators



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- Plus Dirk Nuyens
and Don Zagier, ...


## Dedication: To my friend



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- A remarkable man and a brilliant (physical and computational) scientist and inventor, from Reed College
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- Developer of the Pixar compression format
- and the iPod shuffle
http://en.wikipedia.org/wiki/Richard_Crandall


## Some early conclusions:

Key ideas: randomness, normality of numbers, planar walks, and fractals


## How not to experiment

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Key ideas: randomness, normality of numbers, planar walks, and fractals
Maths can be done experimentally (it is fun)

- using computer algebra, numerical computation and graphics: SNaG
- computations, tables and pictures are experimental data
- but you can not stop thinking

How not to experiment

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When I have clarified and exhausted a subject, then I turn away from it, in order to go into darkness again; the never-satisfied man is so strange if he has completed a structure, then it is not in order to dwell in it peacefully, but in order to begin another.

I imagine the world conqueror must feel thus, who, after one kingdom is scarcely conquered, stretches out his arms for others.


Carl Friedrich Gauss
(1777-1855)

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- In an 1808 letter to his friend Farkas (father of Janos Bolyai)
- Archimedes, Euler, Gauss are the big three


## Walking on Real Numbers

## A Multiple Media Mathematics Project



MOTNATED by the desire to visualize large mathematical data sets，especially in number theory．we offer various tools for re： floating point numbers as planar（or three dimensional）walks and for quantitatively measuring their＂randomness＂．This is ou homepage that discusses and showcases our research．Come back regularly for updates．

RESEARCH TEAM：Francisco 1．Aragon Artacho，David H．Bailey，Jonathan M．Borwein，Peter B．Borwein with the assistance of Ja Fountain and Matt Skerritt．

## CONTACT：EranAragon

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Almost all I mention is accessible at http：／／carma．newcastle．edu．au／walks／

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(1) PART I: Visual Theorems

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(3) PART II. Case Studies
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## Computer Assisted Research Maths: what it is?

Experimental mathematics is the use of a computer to run computations-sometimes no more than trial-and- error tests-to look for patterns, to identify particular numbers and sequences, to gather evidence in support of specific mathematical assertions that may themselves arise by computational means, including search.

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Like contemporary chemists - and before them the alchemists of old-who mix various substances together in a crucible and heat them to a high temperature to see what happens, today's experimental mathematicians put a hopefully potent mix of numbers, formulas, and algorithms into a computer in the hope that something of interest emerges. (JMB-Devlin, Crucible 2008, p. 1)

- Quoted in International Council on Mathematical Instruction

Study 19: On Proof and Proving, 2012

## Experimental Mathematics: Integer Relation Methods

Secure Knowledge without Proof. Given real numbers $\beta, \alpha_{1}, \alpha_{2}, \ldots, \alpha_{n}$, Helaman Ferguson's integer relation method (PSLQ), finds a nontrivial linear relation of the form

$$
\begin{equation*}
a_{0} \beta+a_{1} \alpha_{1}+a_{2} \alpha_{2}+\cdots+a_{n} \alpha_{n}=0 \tag{1}
\end{equation*}
$$

where $a_{i}$ are integers-if one exists and provides an exclusion bound otherwise.


Carving His Own Unique Niche, In Symbols and Stone
By refusing to choose between mathematics and art, a self-described "misfit" has found the place where parallet careers meet

CMS D. Borwein Prize: Madelung


2013 Lattice Sums book (CUP)

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## PSLQ in action

In all serious computations of $\pi$ from 1700 (by John Machin) until 1980 some version of a Machin formula was used. These write

$$
\begin{equation*}
\arctan (1)=a_{1} \cdot \arctan \left(\frac{1}{p_{1}}\right)+a_{2} \cdot \arctan \left(\frac{1}{p_{2}}\right)+\cdots+a_{n} \cdot \arctan \left(\frac{1}{p_{n}}\right) \tag{2}
\end{equation*}
$$

for rationals $a_{1}, a_{2}, \ldots, a_{n}$ and integers $p_{1}, p_{2}, \ldots, p_{n}>1$. Recall the Taylor series $\arctan (x)=\sum_{n=0}^{\infty} \frac{(-1)^{n}}{2 n+1} x^{2 n+1}$. Combined with (2) this computes $\pi=4 \arctan (1)$ efficiently, especially if the $p_{n}$ are not too small.

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For instance, Machin found

$$
\pi=16 \arctan \left(\frac{1}{5}\right)-4 \arctan \left(\frac{1}{239}\right)
$$

while Euler discovered

$$
\begin{equation*}
\arctan (1)=\arctan \left(\frac{1}{2}\right)+\arctan \left(\frac{1}{5}\right)+\arctan \left(\frac{1}{8}\right) \tag{3}
\end{equation*}
$$

## PSLQ in action

In all serious computations of $\pi$ from 1700 (by John Machin) until 1980 some version of a Machin formula was used. These write

$$
\begin{equation*}
\arctan (1)=a_{1} \cdot \arctan \left(\frac{1}{p_{1}}\right)+a_{2} \cdot \arctan \left(\frac{1}{p_{2}}\right)+\cdots+a_{n} \cdot \arctan \left(\frac{1}{p_{n}}\right) \tag{2}
\end{equation*}
$$

for rationals $a_{1}, a_{2}, \ldots, a_{n}$ and integers $p_{1}, p_{2}, \ldots, p_{n}>1$.
Recall the Taylor series $\arctan (x)=\sum_{n=0}^{\infty} \frac{(-1)^{n}}{2 n+1} x^{2 n+1}$. Combined with (2) this computes $\pi=4 \arctan (1)$ efficiently, especially if the $p_{n}$ are not too small.
For instance, Machin found

$$
\pi=16 \arctan \left(\frac{1}{5}\right)-4 \arctan \left(\frac{1}{239}\right)
$$

while Euler discovered

$$
\begin{equation*}
\arctan (1)=\arctan \left(\frac{1}{2}\right)+\arctan \left(\frac{1}{5}\right)+\arctan \left(\frac{1}{8}\right) \tag{3}
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$$

- I have a function 'ps lq' in Maple. When input data for PSLQ it predicts an answer to the precision requested. And checks it to ten digits more (or some other precision).
- This makes the code a real experimental tool as it predicts and confirms.


## PSLQ in action

## prepping for class

- The third shows that when no relation exists the code may find a good approximation but using very large rationals.


## PSLQ in action

```
\(>\operatorname{pslq}(\arctan (1),[\arctan (1 / 2), \arctan (1 / 5), \arctan (1 / 8)], 20) ;\);
                [1, 1, 1, 1], "Error is", 0., "checking to", 30, places
\[
\frac{1}{4} \pi=\arctan \left(\frac{1}{2}\right)+\arctan \left(\frac{1}{5}\right)+\arctan \left(\frac{1}{8}\right)
\]
    pslq(arctan(1), \([\arctan (1 / 2), \arctan (1 / 3), \arctan (1 / 8)], 20) ;\)
    [ \(1,1,1,0]\), "Error is", \(-1.10^{-30}\), "checking to", 30 , places
\[
\frac{1}{4} \pi=\arctan \left(\frac{1}{2}\right)+\arctan \left(\frac{1}{3}\right)
\]
pslq(arctan(1), [arctan(1/2), arctan(1/5), arctan(1/9)],20); [42613, 72375, 22013, -40066], "Error is", \(2.3160464903710^{-15}\), "checking to", 30, places
\[
\frac{1}{4} \pi=\frac{72375}{42613} \arctan \left(\frac{1}{2}\right)+\frac{22013}{42613} \arctan \left(\frac{1}{5}\right)-\frac{40066}{42613} \arctan \left(\frac{1}{9}\right)
\]
pslq(Pi, [arctan \((1 / 5), \arctan (1 / 239)], 20) ;\)
[1, 16, -4], "Error is", \(2.810^{-30}\), "checking to", 30, places
\[
\pi=16 \arctan \left(\frac{1}{5}\right)-4 \arctan \left(\frac{1}{239}\right)
\]
```

- The third shows that when no relation exists the code may find a good approximation but using very large rationals.
- So it diagnoses failure because it uses large coefficients and because it is not true to the requested 30 places.


## Contents

O
PART I: Visual Theorems

- Visual theorems
- Large matrices
- Experimental mathematics
(2) Digital Assistance
- Digital Assistance
- Simulation in Mathematics

O
PART II. Case Studies

- la. Iterated reflections
- lb: Protein conformation
- Ila: 100 digit challenge
- Ilb: Polylogarithms

PART III: Randomness

- Randomness is slippery
- Normality
- Normality of Pi
- BBP Digit Algorithms
- Some background
- Illa. Short rambles

Number walks

- Number walks (base four)


## Walks on 'reals'

- IIIb: Study of number walks
- IIIc: Stoneham numbers
(8) Features of our walks
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- Number of points visited
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## Other realisations

- Fractals everywhere
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- Largely symbolic packages include the commercial computer algebra packages Maple and Mathematica, and the open source SAGE.
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- Specialized Packages or General Purpose Languages such as Fortran, C++, Python, CPLEX, PARI, SnapPea, and MAGMA.


## Digital Assistance

- Web Applications such as: Sloane's Encyclopedia of Integer Sequences, the Inverse Symbolic Calculator, Fractal Explorer, Jeff Weeks' Topological Games, or Euclid in Java. ${ }^{3}$
- Most of the functionality of the ISC is built into the "identify" function Maple starting with version 9.5. For example, identify (4.45033263602792) returns $\sqrt{3}+e$. As always, the experienced will extract more than the novice.

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- Web Databases including Google, MathSciNet, ArXiv, GitHub, Wikipedia, MathWorld, MacTutor, Amazon, Wolfram Alpha, the DLMF (all formulas of which are accessible in MathML, as bitmaps, and in $\mathrm{T}_{\mathrm{E}} \mathrm{X}$ ) and many more that are not always so viewed.

[^7]
## Digital Assistance

All entail data-mining . Franklin argues "exploratory experimentation" facilitated by "widening technology", as in finance, pharmacology, astrophysics, medicine, and biotechnology, is leading to a reassessment of what legitimates experiment; in that a "local model" is not now prerequisite. Sørenson says experimental mathematics is following similar tracks.

These aspects of exploratory experimentation and wide instrumentation originate from the philosophy of (natural) science and have not been much developed in the context of experimental mathematics. However, I claim that e.g. the importance of wide instrumentation for an exploratory approach to experiments that includes concept formation also pertain to mathematics.

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In consequence, boundaries between mathematics and natural sciences and between inductive and deductive reasoning are blurred and getting more so.
I leave the philosophically-vexing if mathematically-minor question as to if genuine mathematical experiments exist even if one embraces a fully idealist notion of mathematical existence. They sure feel like they do.

## Top Ten Algorithms (20C):

## all but one well used in CARMA

## Algorithms for the Ages

"Great algorithms are the poetry of computation," says Francis Sullivan of the Institute for Defense Analyses' Center for Computing Sciences in Bowie, Maryland. He and Jack Dongarra of the University of Tennessee and Oak Ridge National Laboratory have put together a sampling that might have made Robert Frost beam with pride--had the poet been a computer jock. Their list of 10 algorithms having "the greatest influence on the development and practice of science and engineering in the 20th century" appears in the January/February issue of Computing in Science \& Engineering. If you use a computer, some of these algorithms are no doubt crunching your data as you read this. The drum roll, please:

1. 1946: The Metropolis Algorithm for Monte Carlo. Through the use of random processes, this algorithm offers an efficient way to stumble toward answers to problems that are too complicated to solve exactly.
2. 1947: Simplex Method for Linear Programming. An elegant solution to a common problem in planning and decision-making.
3. 1950: Krylov Subspace Iteration Method. A technique for rapidly solving the linear equations that abound in scientific computation.
4. 1951: The Decompositional Approach to Matrix Computations. A suite of techniques for numerical linear algebra.
5. 1957: The Fortran Optimizing Compiler. Turns high-level code into efficient computer-readable code.
6. 1959: QR Algorithm for Computing Eigenvalues. Another crucial matrix operation made swift and practical.
7. 1962: Quicksort Algorithms for Sorting. For the efficient handling of large databases.
8. 1965: Fast Fourier Transform. Perhaps the most ubiquitous algorithm in use today, it breaks down waveforms (like sound) into periodic components.
9. 1977: Integer Relation Detection. A fast method for spotting simple equations satisfied by collections of seemingly unrelated numbers.
10. 1987: Fast Multipole Method. A breakthrough in dealing with the complexity of $n$-body calculations, applied in problems ranging from celestial mechanics to protein folding.

From Random Samples, Science page 799, February 4, 2000.

## Experimental Mathematics: PSLQ is core to CARMA

SECOID EDITION

Ilathematics by Erperiment

Plausible Rensoning in the 2lsi Cemiuhy

Jonalhan Borwein David Bailey

Figure 6.3. Three images quantized at quality $50(\mathrm{~L}), 48$ (C) and 75 (R). Courtesy of Mason Macklem.


Experimentelle Mathematik
fine beicielsrientiote Eintiduras

## Syderym



Experimental Mathematics (2004-08, 2009, 2010)

## Contents

(1)
PART I: Visual Theorems

- Visual theorems
- Large matrices
- Experimental mathematics
(2) Digital Assistance
- Digital Assistance
- Simulation in Mathematics
o
PART II. Case Studies
- la. Iterated reflections
- lb: Protein conformation
- Ila: 100 digit challenge
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PART III: Randomness

- Randomness is slippery
- Normality
- Normality of Pi
- BBP Digit Algorithms
- Some background
- Illa. Short rambles

Number walks

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Walks on 'reals'

- IIIb: Study of number walks
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Features of our walks

- Expected distance to origin
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## Other realisations

- Fractals everywhere
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## Simulation in pure mathematics

Pure mathematicians have not often though of simulation as a relevant tool.
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\begin{equation*}
\mathscr{R}(a, b)=\frac{a}{1+\frac{b^{2}}{1+\frac{4 a^{2}}{1+\frac{9 b^{2}}{1+}}}} . \tag{4}
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We eventually determined from highly sophisticated arguments that:

## Simulation in pure mathematics

Theorem (Six formulae for $\mathscr{R}(a, a), a>0$ )

$$
\begin{aligned}
& \mathscr{R}(a, a)=\int_{0}^{\infty} \frac{\operatorname{sech}\left(\frac{\pi x}{2 a}\right)}{1+x^{2}} \mathrm{~d} x \\
& =2 a \sum_{k=1}^{\infty} \frac{(-1)^{k+1}}{1+(2 k-1) a} \\
& =\frac{1}{2}\left(\psi\left(\frac{3}{4}+\frac{1}{4 a}\right)-\psi\left(\frac{1}{4}+\frac{1}{4 a}\right)\right) \\
& =\frac{2 a}{1+a}{ }_{2} F_{1}\left(\left.\begin{array}{c}
\frac{1}{2 a}+\frac{1}{2}, 1 \\
\frac{1}{2 a}+\frac{3}{2}
\end{array} \right\rvert\,-1\right) \\
& =2 \int_{0}^{1} \frac{t^{1 / a}}{1+t^{2}} \mathrm{~d} t \\
& =\int_{0}^{\infty} e^{-x / a} \operatorname{sech}(x) \mathrm{d} x \text {. }
\end{aligned}
$$

## Simulation in pure mathematics

Here ${ }_{2} F_{1}$ is the hypergeometric function. If you do not know $\psi$ ('psi'), you can easily look it up once you can say 'psi'.
Notice that

$$
\mathscr{R}(a, a)=2 \int_{0}^{1} \frac{t^{1 / a}}{1+t^{2}} \mathrm{~d} t
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so that $R(1,1)=\log 2$.

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- After making no progress analytically, Crandall and I decided in 2003, taking a somewhat arbitrary criterion for convergence, to colour yellow points for which the fraction seemed to converge.
- We sampled one million points and reasoned a few thousand mis-categorisations would not damage the experiment.



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The Figure is so precise that we could identify the cardioid. It is the points where

$$
\sqrt{|a b|} \leq \frac{|a+b|}{2}
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Since for positive $a, b$ the fraction satisfies

$$
\mathscr{R}\left(\frac{a+b}{2}, \sqrt{a b}\right)=\frac{\mathscr{R}(a, b)+\mathscr{R}(b, a)}{2}
$$

this gave us enormous impetus to continue our eventually successful hunt for a proof.

## Contents

OPART I: Visual Theorems

- Visual theorems
- Large matrices
- Experimental mathematics


Digital Assistance

- Digital Assistance
- Simulation in Mathematics
(3) PART II. Case Studies
- la. Iterated reflections
- lb: Protein conformation
- Ila: 100 digit challenge
- Ilb: Polylogarithms

PART III: Randomness

- Randomness is slippery
- Normality
- Normality of Pi
- BBP Digit Algorithms
- Some background
- Illa. Short rambles

Number walks

- Number walks (base four)

Walks on 'reals'

- IIIb: Study of number walks
- IIIc: Stoneham numbers
(8) Features of our walks
- Expected distance to origin
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## Other realisations

- Fractals everywhere
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## Reflection methods

Let $S \subseteq \mathbb{R}^{m}$. The (nearest point or metric) projection onto $S$ is the (set-valued) mapping,

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P_{S} x:=\underset{s \in S}{\arg \min }\|s-x\| .
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The reflection w.r.t. $S$ is the (set-valued) mapping,

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## The Douglas-Rachford Algorithm (1956-1979- )

## Theorem (Douglas-Rachford in finite dimensions)

Suppose $A, B \subseteq \mathbb{R}^{m}$ are closed and convex. For any $x_{0} \in \mathbb{R}^{m}$ define

$$
x_{n+1}:=T_{A, B} x_{n} \text { where } T_{A, B}:=\frac{I+R_{B} R_{A}}{2} .
$$

If $A \cap B \neq \emptyset$, then $x_{n} \rightarrow x$ such that $P_{A} x \in A \cap B$. Else $\left\|x_{n}\right\| \rightarrow+\infty$.


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- http://carma.newcastle.edu.au/jon/expansion.html



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- note the error from using only 14 digit computation.


## Works for $B$ affine and A a 'sphere'

What we could prove (L) and what we could see (R)


## Contents

(1)PART I: Visual Theorems

- Visual theorems
- Large matrices
- Experimental mathematics


Digital Assistance

- Digital Assistance
- Simulation in Mathematics
(3) PART II. Case Studies
- la. Iterated reflections
- lb: Protein conformation
- Ila: 100 digit challenge
- Ilb: Polylogarithms

PART III: Randomness

- Randomness is slippery
- Normality
- Normality of Pi
- BBP Digit Algorithms
- Some background
- Illa. Short rambles

Number walks

- Number walks (base four)


## Walks on 'reals'

- IIIb: Study of number walks
- IIIc: Stoneham numbers

Features of our walks

- Expected distance to origin
- Number of points visited
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## Other realisations

- Fractals everywhere
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- References


## Case study I: Protein conformation determination

Proteins: large biomolecules comprising multiple amino acid chains. ${ }^{4}$


Generic amino acid


RuBisCO


Matt Tam

[^8]
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A low-rank Euclidean distance matrix completion problem.

[^10]
## Six Proteins

We use only interatomic distances below 6Å typically constituting less than $8 \%$ of the total nonzero entries of the distance matrix.

Table. Six Proteins: average (maximum) errors from five replications.

| Protein | \# Atoms | Rel. Error (dB) | RMSE | Max Error |
| :---: | :---: | :---: | :---: | :---: |
| 1PTQ | 404 | $-83.6(-83.7)$ | $0.0200(0.0219)$ | $0.0802(0.0923)$ |
| 1HOE | 581 | $-72.7(-69.3)$ | $0.191(0.257)$ | $2.88(5.49)$ |
| 1LFB | 641 | $-47.6(-45.3)$ | $3.24(3.53)$ | $21.7(24.0)$ |
| 1PHT | 988 | $-60.5(-58.1)$ | $1.03(1.18)$ | $12.7(13.8)$ |
| 1POA | 1067 | $-49.3(-48.1)$ | $34.1(34.3)$ | $81.9(87.6)$ |
| 1AX8 | 1074 | $-46.7(-43.5)$ | $9.69(10.36)$ | $58.6(62.6)$ |

$$
\begin{gathered}
\text { Rel. } \operatorname{error}(d B):=10 \log _{10}\left(\frac{\left\|P_{C_{2}} P_{C_{1}} X_{N}-P_{C_{1}} X_{N}\right\|^{2}}{\left\|P_{C_{1}} X_{N}\right\|^{2}}\right), \\
\text { RMSE }:=\sqrt{\frac{\sum_{i=1}^{m}\left\|\hat{p}_{i}-p_{i}^{\text {true }}\right\|_{2}^{2}}{\# \text { of atoms }}}, \quad \operatorname{Max}:=\max _{1 \leq i \leq m}\left\|\hat{p}_{i}-p_{i}^{\text {true }}\right\|_{2} .
\end{gathered}
$$

- The points $\hat{p}_{1}, \hat{p}_{2}, \ldots, \hat{p}_{n}$ denote the best fitting of $p_{1}, p_{2}, \ldots, p_{n}$ when rotation, translation and reflection is allowed.


## What do the reconstructions look like?



1PTQ (actual)

1POA (actual)


5,000 steps, -83.6 dB (perfect)


5,000 steps, -49.3 dB (mainly good!)

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- The picture of 'failure' suggests many strategies


## What do reconstructions look like?



Iterations: 4
Video: First 3,000 steps of the 1PTQ reconstruction.
At http://carma.newcastle.edu.au/DRmethods/1PTQ.html

## What do the Reconstructions Look Like?

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Figure: Relative error by iterations (vertical axis logarithmic).

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Figure: Relative error by iterations (vertical axis logarithmic).

- For $<5,000$ iterations, the error exhibits non-monotone oscillatory behaviour. It then decreases sharply. Beyond this progress is slower.
- Is early termination to blame? Terminate when error $<-100 \mathrm{~dB}$.


## A More Robust Stopping Criterion

The "un-tuned" implementation (from previous slide):


1POA (actual)


5,000 steps (~2d), -49.3dB

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28,500 steps ( $\sim 1 d$ ), -100 dB (perfect!)

Q Similar results observed for the other test oroteins.

## What do reconstructions look like?

There are many projection methods, so why use Douglas-Rachford?
Douglas-Rachford reflection method reconstruction:


500 steps, -25 dB .


1,000 steps, -30 dB .


2,000 steps, -51 dB .


5,000 steps, -84 dB .

Alternating projection method reconstruction:


500 steps, -22 dB .


1,000 steps, -24 dB .


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- Yet MAP works very well for optical abberation correction (Hubble, amateur telescopes).


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(1)PART I: Visual Theorems

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- Large matrices
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Digital Assistance

- Digital Assistance
- Simulation in Mathematics
(3) PART II. Case Studies
- la. Iterated reflections
- lb: Protein conformation
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PART III: Randomness

- Randomness is slippery
- Normality
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Number walks

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## Walks on 'reals'

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## How the mathematical software world has changed

In the January 2002 issue of SIAM News, Nick Trefethen presented ten diverse problems used in teaching modern graduate numerical analysis students at Oxford University, the answer to each being a certain real number.

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"If anyone gets 50 digits in total, I will be impressed."

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"If anyone gets 50 digits in total, I will be impressed."

- To his surprise, a total of 94 teams, representing 25 different nations, submitted results. Twenty of these teams received a full 100 points (10 correct digits for each problem).
- Bailey, Fee and I quit at 85 digits!


## The hundred digit challenge

The problems and solutions are dissected most entertainingly in [1] F. Bornemann, D. Laurie, S. Wagon, and J. Waldvogel (2004)."The Siam 100-Digit Challenge: A Study In High-accuracy Numerical Computing", SIAM, Philadelphia.

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Success in solving these problems required a broad knowledge of mathematics and numerical analysis, together with significant computational effort, to obtain solutions and ensure correctness of the results. As described in [1] the strengths and limitations of Maple, Mathematica, MATLAB (The 3Ms), and other software tools such as PARI or GAP, were strikingly revealed in these ventures.

Almost all of the solvers relied in large part on one or more of these three packages, and while most solvers attempted to confirm their results, there was no explicit requirement for proofs to be provided.

## Trefethen's problem \#9

The integral
$I(\alpha)=\int_{0}^{2}[2+\sin (10 \alpha)] x^{\alpha} \sin \left(\frac{\alpha}{2-x}\right) \mathrm{d} x$
depends on the parameter $\alpha$. What is the value $\alpha \in[0,5]$ at which $I(\alpha)$ achieves its maximum?


Integrands for some $\alpha$

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Integrands for some $\alpha$

- $I(\alpha)$ is expressible in terms of a Meijer-G function -a special function with a solid history that we use below.
- Unlike most contestants, Mathematica and Maple will figure this out; help files or a web search then inform the scientist.
- This is another measure of the changing environment. It is usually a good idea-and not at all immoral-to data-mine.


## Trefethen's problem \#10

A particle at the center of a $10 \times 1$ rectangle undergoes Brownian motion (i.e., 2-D random walk with infinitesimal step lengths) till it hits the boundary. What is the probability that it hits at one of the ends rather than at one of the sides?

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A particle at the center of a $10 \times 1$ rectangle undergoes Brownian motion (i.e., 2-D random walk with infinitesimal step lengths) till it hits the boundary. What is the probability that it hits at one of the ends rather than at one of the sides?

Hitting the Ends. Bornemann [1] starts his remarkable solution by exploring Monte-Carlo methods, which are shown to be impracticable.

- He reformulates the problem deterministically as the value at the center of a $10 \times 1$ rectangle of an appropriate harmonic measure of the ends, arising from a 5-point discretization of Laplace's equation with Dirichlet boundary conditions.
- This is then solved by a well chosen sparse Cholesky solver. A reliable numerical value of $3.837587979 \cdot 10^{-7}$ is obtained and the problem is solved numerically to the requisite ten places.
- This is the warm up....


## Walking in a $b \times a$ box



## Trefethen's problem \#10

We may proceed to develop two analytic solutions, the first using separation of variables on the underlying PDE on a general $2 a \times 2 b$ rectangle. We learn that with $\rho:=a / b$

$$
\begin{equation*}
p(a, b)=\frac{4}{\pi} \sum_{n=0}^{\infty} \frac{(-1)^{n}}{2 n+1} \operatorname{sech}\left(\frac{\pi(2 n+1)}{2} \rho\right) \tag{5}
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$$

- Three terms yields 50 correct digits:

$$
p(10,1)=\underline{0.0000003837587979} 2512261034071331862048391007930055940724 \ldots
$$

- The first term alone, $\frac{4}{\pi} \operatorname{sech}(5 \pi)$, gives the underlined digits.


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$$

- The first term alone, $\frac{4}{\pi} \operatorname{sech}(5 \pi)$, gives the underlined digits.

A second method using conformal mappings, yields

$$
\begin{equation*}
\operatorname{arccot} \rho=p(a, b) \frac{\pi}{2}+\arg \mathrm{K}\left(e^{i p(a, b) \pi}\right) \tag{6}
\end{equation*}
$$

where K is the complete elliptic integral of the first kind.

## Trefethen's problem \#10

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- We have entered the wonderful world of modular functions Bornemann et al ultimately show that the answer is

$$
\begin{equation*}
p=\frac{2}{\pi} \arcsin \left(k_{100}\right) \tag{7}
\end{equation*}
$$

where

$$
k_{100}:=\left((3-2 \sqrt{2})(2+\sqrt{5})(-3+\sqrt{10})(-\sqrt{2}+\sqrt[4]{5})^{2}\right)^{2}
$$

is a singular value. [In general $p(a, b)=\frac{2}{\pi} \arcsin \left(k_{(a / b)^{2}}\right)$.]

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is a singular value. [In general $p(a, b)=\frac{2}{\pi} \arcsin \left(k_{(a / b)^{2}}\right)$.]

- No one (except harmonic analysts perhaps) anticipated a closed form-let alone one like this.
- Can be done for some other shapes (perhaps, convex with piecewise smooth boundaries, starting at barycentre), and for self-avoiding walks.


## Trefethen's problem \#4

## What is the global minimum of the function

$\exp (\sin (50 x))+\sin \left(60 e^{y}\right)+\sin (70 \sin x)+\sin (\sin (80 y))$

$$
-\sin (10(x+y))+\left(x^{2}+y^{2}\right) / 4 ?
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$$
-\sin (10(x+y))+\left(x^{2}+y^{2}\right) / 4 ?
$$



- Can be solved in a global optimization package or by a damped Newton method
- In Mathematica by NMinimize[f[x, y], x, y, Method -> "RandomSearch", "SearchPoints" -> 250, WorkingPrecision -> 20]
- In Maple by NLPSolve ( $\mathrm{f}(\mathrm{x}, \mathrm{y})$, $\mathrm{x}=-4 . .4, \mathrm{y}=-4$.. 4, initialpoint $=\{\mathrm{x}=-.4, \mathrm{y}=-.1\}$ );
- or by 'zooming' on $[-3,3] \times[-3,3]$.


## Trefethen's problem \#4



## Contents

(1)PART I: Visual Theorems

- Visual theorems
- Large matrices
- Experimental mathematics


Digital Assistance

- Digital Assistance
- Simulation in Mathematics
(3) PART II. Case Studies
- Ia. Iterated reflections
- lb: Protein conformation
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PART III: Randomness

- Randomness is slippery
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- Some background
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Number walks

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## Walks on 'reals'

- IIIb: Study of number walks
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## Features of our walks

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## Algorithm performance

## Proposition (Polylogarithm computation)

(a) For $s=n$ a positive integer,

$$
\begin{equation*}
\operatorname{Li}_{n}(z)=\sum_{m=0}^{\infty} \zeta(n-m) \frac{\log ^{m} z}{m!}+\frac{\log ^{n-1} z}{(n-1)!}\left(H_{n-1}-\log (-\log z)\right) . \tag{8}
\end{equation*}
$$

(b) For any complex order s not a positive integer,

$$
\begin{equation*}
\operatorname{Li}_{s}(z)=\sum_{m \geq 0} \zeta(s-m) \frac{\log ^{m} z}{m!}+\Gamma(1-s)(-\log z)^{s-1} \tag{9}
\end{equation*}
$$

Here $\zeta(s):=\sum_{n}^{-s}$ and continuations, $H_{n}:=1+\frac{1}{2}+\frac{1}{3}+\cdots+\frac{1}{n}$, and $\Sigma^{\prime}$ avoids the singularity at $\zeta(1)$. In (8), $|\log z|<2 \pi$ precludes use when $|z|<e^{-2 \pi} \approx 0.0018674$. For small $|z|$, however, it suffices to use the definition

$$
\operatorname{Li}_{s}(z)=\sum_{k=1}^{\infty} \frac{z^{k}}{k^{s}} .
$$

## Algorithm performance

- We found (10) faster than (8) whenever $|z|<1 / 4$, for precision from 100 to 4000 digits. We illustrate for $\mathrm{Li}_{2}$ in the Figure.



Figure: (L) Timing (8) (blue) and (10) (red).(R) blue region where (8) is faster.

## Algorithm performance

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- Timings show microseconds required for 1,000 digit accuracy as the modulus goes from 0 to 1 with blue showing superior performance of (8). The region records 10,000 trials of random $z$, such that $-0.6<\mathfrak{R}(z)<0.4,-0.5<\mathfrak{I}(z)<0.5$.



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PART I: Visual Theorems

- Visual theorems
- Large matrices
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Digital Assistance

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- Simulation in Mathematics


PART II. Case Studies

- la. Iterated reflections
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4 PART III: Randomness

- Randomness is slippery
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## We shall explore things like:

Remember: $\pi$ is area of a circle of radius one (and perimeter is $2 \pi$ ).

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First true calculation of $\pi$ was due to Archimedes of Syracuse (287-212 BCE). He used a brilliant scheme for doubling inscribed and circumscribed polygons (with 'interval arithmetic')


$$
\begin{gathered}
\mathbf{6} \mapsto \mathbf{1 2} \mapsto 24 \mapsto 48 \mapsto \mathbf{9 6} \text { to obtain the estimate } \\
3 \frac{10}{71}<\pi<3 \frac{10}{70} .
\end{gathered}
$$

## Archimedes' "Method of Mechanical Theorems"

Pi movie below

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Pi movie below
... certain things first became clear to me by a mechanical method (Codex C), although they had to be proved by geometry afterwards because their investigation by the said method did not furnish an actual proof.

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But it is of course easier, when we have previously acquired, by the method, some knowledge of the questions, to supply the proof than it is to find it without any previous knowledge.

- Only recently rediscovered and even more recently reconstructed ...


## Proving $\pi$ is not $\frac{22}{7}$

Even Maple or Mathematica 'knows' this since

$$
\begin{equation*}
0<\int_{0}^{1} \frac{(1-x)^{4} x^{4}}{1+x^{2}} d x=\frac{22}{7}-\pi, \tag{11}
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- Accidentally, $22 / 7$ is one of the early continued fraction approximation to $\pi$. These commence:

$$
3, \frac{22}{7}, \frac{333}{106}, \frac{355}{113}, \ldots
$$

## Proving $\pi$ is not $\frac{22}{7}$

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## Proving $\pi$ is not $\frac{22}{7}$

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We obtain

$$
\int_{0}^{t} \frac{x^{4}(1-x)^{4}}{1+x^{2}} d x=\frac{1}{7} t^{7}-\frac{2}{3} t^{6}+t^{5}-\frac{4}{3} t^{3}+4 t-4 \arctan (t)
$$

as differentiation easily confirms, and the fundamental theorem of calculus proves (11).

An opinion without 3.14 is an onion. You'll understand.

## Randomness

- The digits expansions of $\pi, e, \sqrt{2}$ appear to be "random":

$$
\begin{aligned}
\pi & =3.141592653589793238462643383279502884197169399375 \ldots \\
e & =2.718281828459045235360287471352662497757247093699 \ldots \\
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$$

## Are they really?

- 1949 ENIAC (Electronic Numerical Integrator and Calculator) computed of $\pi$ to 2,037 decimals (in 70 hours) -proposed by polymath John von Neumann (1903-1957) to shed light on distribution of $\pi$ (and of $e$ ).



## Two continued fractions

## Change representations often

Gauss map. Remove the integer, invert the fraction and repeat: for 3.1415926 and 2.7182818 to get the fractions below.


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Gauss map. Remove the integer, invert the fraction and repeat: for 3.1415926 and 2.7182818 to get the fractions below.


Leonhard Euler (17071783) named $e$ and $\pi$.
"Lisez Euler, lisez Euler, c'est notre maître à tous." Simon Laplace (1749-1827)

## Are the digits of $\pi$ random?

| Digit | Ocurrences |
| :---: | ---: |
| 0 | $99,993,942$ |
| 1 | $99,997,334$ |
| 2 | $100,002,410$ |
| 3 | $99,986,911$ |
| 4 | $100,011,958$ |
| 5 | $99,998,885$ |
| 6 | $100,010,387$ |
| 7 | $99,996,061$ |
| 8 | $100,001,839$ |
| 9 | $100,000,273$ |
| Total | $\mathbf{1 , 0 0 0}, \mathbf{0 0 0}, \mathbf{0 0 0}$ |

Table: Counts of first billion digits of $\pi$. Second half is 'right' for law of large
numbers.

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Table: Counts of first billion digits of $\pi$. Second half is 'right' for law of large numbers.

Pi is Still Mysterious. We know $\pi$ is not algebraic; but do not 'know' (in sense of being able to prove) whether ....

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- There are infinitely many sevens in the decimal expansion of $\pi$
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- Or pretty much anything else...


## What is "random"?

## A hard question



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## A hard question



It might be:

- Unpredictable (fair dice or coin-flips)?
- Without structure (noise)?
- Algorithmically random ( $\pi$ is not)?
- Quantum random (radiation)?
- Incompressible ('zip’ does not help)?


## What is "random"?

## A hard question

| TOUR OF ACCOUNTING |  | ARE |
| :---: | :---: | :---: |
| OVER HERE WE HAVE OUR RANDOM NUMBER GENERATOR. | NINE NINE NINE NINE |  |

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Conjecture (Borel) All irrational algebraic numbers are $b$-normal

Best Theorem [BBCP, 04] (Feeble but hard) Asymptotically all degree $d$ algebraics have at least $n^{1 / d}$ ones in binary (should be $n / 2$ )

## Randomness in Pi?

http://mkweb.bcgsc.ca/pi/art/


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```
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```



- a better color palette for art if not for science


## Contents

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- Digital Assistance
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(3) PART II. Case Studies
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- Randomness is slippery
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Number walks

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## Walks on 'reals'

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(8) Features of our walks
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## Other realisations

- Fractals everywhere
- 3D drunkard's walks
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## Normality

## Definition

A real constant $\alpha$ is $b$-normal if, given the positive integer $b \geq 2$ (the base), every $m$-long string of base- $b$ digits appears in the base- $b$ expansion of $\alpha$ with precisely the expected limiting frequency $1 / b^{m}$.

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- Given an integer $b \geq 2$, almost all real numbers, with probability one, are $b$-normal (Borel).
- Indeed, almost all real numbers are $b$-normal simultaneously for all positive integer bases ("absolute normality").
- Unfortunately, it has been very difficult to prove normality for any number in a given base $b$, much less all bases simultaneously.



## Normal numbers

## concatenation numbers

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C_{10}:=0.123456789101112131415161718 \ldots
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C E(10):=0.23571113171923293137414347 \ldots
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- Normality proofs are not known for $\pi, e, \log 2, \sqrt{2}$ etc.


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## Theorem (Davenport-Erdös (1952))

Let $p$ be any polynomial positive on the natural numbers. Then the concatenation number

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0 . p(1) p(2) p(3) \ldots p(n) \ldots
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is Borel normal (in the base of presentation).

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- Includes Champernowne's number and 0.1491625... (Besicovich)
- See H. Davenport and P. Erdös, "Note on normal numbers." Can. J. Math., 4 (1952), 58-63.


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(1)PART I: Visual Theorems

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- Experimental mathematics


Digital Assistance

- Digital Assistance
- Simulation in Mathematics
(3) PART II. Case Studies
- la. Iterated reflections
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## - Normality of Pi

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| 0 | $99,993,942$ | 00 | $10,004,524$ | 000 | $1,000,897$ |
| 1 | $99,997,334$ | 01 | $9,998,250$ | 001 | $1,00,758$ |
| 2 | $100,002,410$ | 02 | $9,999,222$ | 002 | $1,000,447$ |
| 3 | $99,986,911$ | 03 | $10,000,290$ | 003 | $1,001,566$ |
| 4 | $100,011,958$ | 04 | $10,000,613$ | 004 | $1,000,741$ |
| 5 | $99,998,885$ | 05 | $10,002,048$ | 005 | $1,002,881$ |
| 6 | $100,010,387$ | 06 | $9,995,451$ | 006 | 999,294 |
| 7 | $99,996,061$ | 07 | $9,993,703$ | 007 | 998,919 |
| 8 | $100,001,839$ | 08 | $10,000,565$ | 008 | 999,962 |
| 9 | $100,000,273$ | 09 | $9,999,276$ | 009 | 999,059 |
|  |  | 10 | $9,997,289$ | 010 | 998,884 |
|  |  | 11 | $9,997,964$ | 011 | $1,001,188$ |
|  |  | $\vdots$ | $\vdots$ | $\vdots$ | $\vdots$ |
|  |  | 99 | $10,003,709$ | 099 | 999,201 |
|  |  |  |  | $\vdots$ | $\vdots$ |
|  |  |  |  | 999 | $1,000,905$ |
| TOTAL | $1,000,000,000$ | TOTAL | $1,000,000,000$ | TOTAL | $1,000,000,000$ |

Table: Counts for the first billion digits of $\pi$.

## Is $\pi$ 16-normal

$\hookleftarrow$ Counts of first trillion hex digits

| 0 | 62499881108 |
| :---: | ---: |
| 1 | 62500212206 |
| 2 | 62499924780 |
| 3 | 62500188844 |
| 4 | 62499807368 |
| 5 | 62500007205 |
| 6 | 62499925426 |
| 7 | 62499878794 |
| 8 | $\underline{\mathbf{6 2 5 0 0 2} 16752}$ |
| 9 | 62500120671 |
| A | 62500266095 |
| B | 62499955595 |
| C | 62500188610 |
| D | 62499613666 |
| E | 62499875079 |
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- They are 353CB3F7F0C9ACCFA9AA215F2

See www.karrels.org/pi/index.html
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OCTOPI

## Modern $\pi$ Calculation Records:

| Name | Year | Correct Digits |
| :--- | :---: | :---: |
| Miyoshi and Kanada | 1981 | $2,000,036$ |
| Kanada-Yoshino-Tamura | 1982 | $16,777,206$ |
| Gosper | 1985 | $17,526,200$ |
| Bailey | Jan. 1986 | $29,360,111$ |
| Kanada and Tamura | Sep. 1986 | $33,554,414$ |
| Kanada and Tamura | Oct. 1986 | $67,108,839$ |
| Kanada et. al | Jan. 1987 | $134,217,700$ |
| Kanada and Tamura | Jan. 1988 | $201,326,551$ |
| Chudnovskys | May 1989 | $480,000,000$ |
| Kanada and Tamura | Jul. 1989 | $536,870,898$ |
| Kanada and Tamura | Nov. 1989 | $1,073,741,799$ |
| Chudnovskys | Aug. 1991 | $2,260,000,000$ |
| Chudnovskys | May 1994 | $4,044,000,000$ |
| Kanada and Takahashi | Oct. 1995 | $6,442,450,938$ |
| Kanada and Takahashi | Jul. 1997 | $51,539,600,000$ |
| Kanada and Takahashi | Sep. 1999 | $206,158,430,000$ |
| Kanada-Ushiro-Kuroda | Dec. 2002 | $1,241,100,000,000$ |
| Takahashi | Jan. 2009 | $1,649,000,000,000$ |
| Takahashi | April 2009 | $2,576,980,377,524$ |
| Bellard | Dec. 2009 | $2,699,999,990,000$ |
| Kondo and Yee | Aug. 2010 | $\mathbf{5 , 0 0 0 , 0 0 0 , 0 0 0 , 0 0 0}$ |
| Kondo and Yee | Oct. 2011 | $\mathbf{1 0 , 0 0 0 , 0 0 0 , 0 0 0 , 0 0 0}$ |
| Kondo and Yee | Dec. 2013 | $\mathbf{1 2 , 1 0 0 , 0 0 0 , 0 0 0 , 0 0 0}$ |



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## What BBP Does?

Prior to 1996, most folks thought to compute the $d$-th digit of $\pi$, you had to generate the (order of) the entire first $d$ digits. This is not true:

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- a computational cost growing only slightly faster than the digit position.
- An algorithm found by computer-now used to check record $\pi$ computations and in some compilers.

This is based on the following then new formula for $\pi$ :

$$
\begin{equation*}
\pi=\sum_{i=0}^{\infty} \frac{1}{16^{i}}\left(\frac{4}{8 i+1}-\frac{2}{8 i+4}-\frac{1}{8 i+5}-\frac{1}{8 i+6}\right) \tag{12}
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\pi=\sum_{i=0}^{\infty} \frac{1}{16^{i}}\left(\frac{4}{8 i+1}-\frac{2}{8 i+4}-\frac{1}{8 i+5}-\frac{1}{8 i+6}\right) \tag{12}
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$$

- Millionth hex digit (four millionth bit) takes under 30 secs on a fairly new PC in Maple (not C++ or Python) and billionth 10 hrs.

Equation (12) was discovered numerically using integer relation methods over months in my BC lab, CECM. It arrived coded as:

## What BBP Is?

This is based on the following then new formula for $\pi$ :

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\pi=4_{2} \mathrm{~F}_{1}\left(1, \frac{1}{4} ; \frac{5}{4},-\frac{1}{4}\right)+2 \tan ^{-1}\left(\frac{1}{2}\right)-\log 5
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where ${ }_{2} \mathrm{~F}_{1}(1,1 / 4 ; 5 / 4,-1 / 4)=0.955933837 \ldots$ is a Gaussian hypergeometric function.

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- Bailey-Crandall (220) link BBP and normality.


## Edge of Computation Prize Finalist (2005)

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- Won by David Deutsch — discoverer of Quantum Computing.


## Stefan Banach (1892-1945) Another Nazi casuality

A mathematician is a person who can find analogies between theorems; a better mathematician is one who can see analogies between proofs and the best mathematician can notice analogies between theories. ${ }^{6}$


[^11]
## Contents

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- Experimental mathematics


Digital Assistance

- Digital Assistance
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- lb: Protein conformation
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- Normality of Pi
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## - Some background

- Illa. Short rambles

Number walks

- Number walks (base four)


## Walks on 'reals'

- IIIb: Study of number walks
- IIIc: Stoneham numbers
(3) Features of our walks
- Expected distance to origin
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(9) Other realisations
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L: Pearson posed question about a 'rambler' taking unit random steps (Nature, '05).

R: Rayleigh gave large $n$ estimates of density: $p_{n}(x) \sim \frac{2 x}{n} e^{-x^{2} / n}$ (Nature, 1905) with $n=5,8$ shown above.

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- appear in graph theory, quantum chemistry, in quantum physics as hexaonnal and diamond lattice integers. etc


## The first walk (Venn)

## Why is the sky blue?



The first person to visualize the random nature of pi's decimal digits was the Victorian nathematician John Venn. In The Logic of Chance (1888), he suggested that the digits 0 to 7 epresent eight compass directions, and he followed the path tracked by these digits in pi. He nisses out the initial 3, and starts 14159. Venn's image was the first "random walk", an idea now ised frequently in probability and statistics. (The illustration is taken from my book, Alex's tdventures in Numberland)


MY HOBBY: TEACHING TRICKY QUESTIONS TO THE CHILDREN OF MY SCIENTIST FRIENDS.

## One 1500-step ramble: a familiar picture



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- 1D (and 3D) easy. Expectation of RMS distance is easy $(\sqrt{n})$.


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- 1D (and 3D) easy. Expectation of RMS distance is easy $(\sqrt{n})$.
- 1D or 2D lattice: probability one of returning to the origin.


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## Case study II: short rambles



1000 three-step uniform planar walks

## The moments of an $n$-step planar walk:

- Second simplest case:

$$
W_{2}=\int_{0}^{1} \int_{0}^{1}\left|e^{2 \pi i x}+e^{2 \pi i y}\right| \mathrm{d} x \mathrm{~d} y=?
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- Mathematica 10 and Maple 18 still think the answer is 0 ('bug' or 'feature'?).


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- There is always a 1-dimension reduction ${ }^{7}$

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\begin{aligned}
W_{n}(s) & =\int_{[0,1]^{n}}\left|\sum_{k=1}^{n} e^{2 \pi x_{k} i}\right|^{s} \mathrm{~d}\left(x_{1}, \ldots, x_{n-1}, x_{n}\right) \\
& =\int_{[0,1]^{n-1}}\left|1+\sum_{k=1}^{n-1} e^{2 \pi x_{k} i}\right|^{s} \mathrm{~d}\left(x_{1}, \ldots, x_{n-1}\right)
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\end{aligned}
$$

- So $W_{2}=4 \int_{0}^{1 / 4} \cos (\pi x) \mathrm{d} x=\frac{4}{\pi}$.


## Art meets science



A visualization of six routes that 1000 ants took after leaving their nest in search of food. The jagged blue lines represent the breaking off of random ants in search of seeds.
(Nadia Whitehead 2014-03-25 16:15)

## Art meets science

## AAAS \& Bridges conference

(JonFest 2011 Logo) Three-step random walks. The (purple) expected distance travelled is 1.57459 ..

The closed form $W_{3}$ is given below.


## Simulating the densities for $n=3,4$



## The radial densities forminn



5-Step Radial Random Walk Probability Density
for $1,000,000$ Trials Allocated to 1,000 Radius Bins


Radius

## (simulations by A. Mattingly)

4-Step Radial Random Walk Probability Density for 1,000,000 Trials Allocated to 1,000 Radius Bins


6-Step Radial Random Walk Probability Density
for 1,000,000 Trials Allocated to 1,000 Radius Bins


## Pearson's original full question

A man starts from a point $O$ and walks $l$ yards in a straight line; he then turns through any angle whatever and walks another $l$ yards in a second straight line. He repeats this process $n$ times. I require the probability that after these $n$ stretches he is at a distance between $r$ and $r+\delta r$ from his starting point, $O$.

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- 2015. Our analysis of short walks extends interestingly to arbitrary dimensions ...


## The radial densities for $n=3,4$ are modular functions

Let $\sigma(x):=\frac{3-x}{1+x}$. Then $\sigma$ is an involution on $[0,3]$ sending $[0,1]$ to $[1,3]$ :

$$
\begin{equation*}
p_{3}(x)=\frac{4 x}{(3-x)(x+1)} p_{3}(\sigma(x)) . \tag{13}
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So $\frac{3}{4} p_{3}^{\prime}(0)=p_{3}(3)=\frac{\sqrt{3}}{2 \pi}, p(1)=\infty$.

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So $\frac{3}{4} p_{3}^{\prime}(0)=p_{3}(3)=\frac{\sqrt{3}}{2 \pi}, p(1)=\infty$. We found:

$$
p_{3}(\alpha)=\frac{2 \sqrt{3} \alpha}{\pi\left(3+\alpha^{2}\right)}{ }_{2} F_{1}\left(\begin{array}{c}
\frac{1}{3}, \frac{2}{3} \\
1
\end{array} \left\lvert\, \frac{\alpha^{2}\left(9-\alpha^{2}\right)^{2}}{\left(3+\alpha^{2}\right)^{3}}\right.\right)=\frac{2 \sqrt{3}}{\pi} \frac{\alpha}{\mathrm{AG}_{3}\left(3+\alpha^{2}, 3\left(1-\alpha^{2}\right)^{2 / 3}\right)}
$$

where $\mathrm{AG}_{3}$ is the cubically convergent mean iteration (1991):

$$
\mathrm{AG}_{3}(a, b):=\frac{a+2 b}{3} \otimes\left(b \cdot \frac{a^{2}+a b+b^{2}}{3}\right)^{1 / 3}
$$

The densities $p_{3}(\mathrm{~L})$ and $p_{4}(\mathrm{R})$

## Formula for the 'shark-fin' $p_{4}$

We ultimately deduce on $2 \leq \alpha \leq 4$ a hyper-closed form:

$$
p_{4}(\alpha)=\frac{2}{\pi^{2}} \frac{\sqrt{16-\alpha^{2}}}{\alpha}{ }_{3} F_{2}\left(\left.\begin{array}{c}
\frac{1}{2}, \frac{1}{2}, \frac{1}{2}  \tag{15}\\
\frac{5}{6}, \frac{7}{6}
\end{array} \right\rvert\, \frac{\left(16-\alpha^{2}\right)^{3}}{108 \alpha^{4}}\right) .
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$\leftarrow p_{4}$ from (15) vs 18 -terms of empirical power series

$$
\begin{aligned}
& \checkmark \text { Proves } p_{4}(2)=\frac{2^{7 / 3} \pi}{3 \sqrt{3}} \Gamma\left(\frac{2}{3}\right)^{-6}= \\
& \frac{\sqrt{3}}{\pi} W_{3}(-1) \approx 0.494233<\frac{1}{2}
\end{aligned}
$$

- Empirically, quite marvelously, we found - and proved by a subtle use of distributional Mellin transforms - that on $[0,2]$ as well:

$$
p_{4}(\alpha) \stackrel{?}{=} \frac{2}{\pi^{2}} \frac{\sqrt{16-\alpha^{2}}}{\alpha} \Re_{3} F_{2}\left(\left.\begin{array}{c}
\frac{1}{2}, \frac{1}{2}, \frac{1}{2}  \tag{16}\\
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$$

(Discovering this $\Re$ brought us full circle.)

## The radial densities for $5 \leq n \leq 8$

## (and large $n$ approximation)






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(and large $n$ approximation)



Both $p_{2 n+4}, p_{2 n+5}$ are $n$-times continuously differentiable for $x>0$ with $p_{n}(x) \sim \frac{2 x}{n} e^{-x^{2} / n}$.


So "four is small" but "eight is large."


## The radial densities for $5 \leq n \leq 8$




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- Pearson wondered if $p_{5}$ was linear on $[0,1]$. Only disproven in sixties.


## Meijer-G (1936) form for $W_{3}$

## Theorem (Meijer-G form for $W_{3}$ )

For $s$ not an odd integer

$$
W_{3}(s)=\frac{\Gamma\left(1+\frac{s}{2}\right)}{\sqrt{\pi} \Gamma\left(-\frac{s}{2}\right)} G_{33}^{21}\left(\begin{array}{c|c}
1,1,1 \\
\frac{1}{2},-\frac{s}{2},-\frac{s}{2} & \frac{1}{4}
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- First found by Crandall via CAS.
- Proved using residue calculus methods.
- $W_{3}(s)$ is among the first non-trivial higher order Meijer-G function to be placed in closed form.



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W_{4}(s)=\frac{2^{s}}{\pi} \frac{\Gamma\left(1+\frac{s}{2}\right)}{\Gamma\left(-\frac{s}{2}\right)} G_{44}^{22}\left(\left.\begin{array}{c}
1, \frac{1-s}{2}, 1,1  \tag{17}\\
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He [Gauss (or Mathematica)] is like the fox, who effaces his tracks in the sand with his tail.— Niels Abel (1802-1829)

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But we really need a formula with $s=1$, that is an integer.

## Visualizing $W_{4}, W_{5}$, and $W_{6}$ on the real line




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- Use recursion from $s>1$


## Visualizing $W_{4}, W_{5}$, and $W_{6}$ on the real line




- Use recursion from $s>1$
- Nonnegativity of $W_{4}$ was hard to prove (Wan)


## Visualizing $W_{4}$ in the complex plane



## Visualizing $W_{4}$ in the complex plane



- Easily drawn now in Mathematica from the Meijer-G representation


## Visualizing $W_{4}$ in the complex plane



- Easily drawn now in Mathematica from the Meijer-G representation
- Each point is coloured differently (black is zero and white infinity). Note the poles and zeros.


## Visualizing $W_{4}$ in the complex plane:



- Easily drawn now in Mathematica from the Meijer-G representation.
- Each quadrant is coloured differently (black is zero and white infinity). Note the poles and zeros.


## Visualizing $W_{4}$ in the complex plane:



- Less easily drawn now from the Meijer-G representation.
- As prepared for Springer's Mathematical Beauties (2016).


## Simplifying the Meijer integrals for $W_{3}$ and $W_{4}$

- We (humans and/or computers) now obtained:


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Corollary (Hypergeometric forms for non-integer $s>-2$ )

$$
\begin{aligned}
& W_{3}(s)=\frac{\tan \left(\frac{\pi s}{2}\right)}{2^{2 s+1}}\binom{s}{\frac{s-1}{2}}^{2}{ }_{3} F_{2}\left(\left.\begin{array}{c}
\frac{1}{2}, \frac{1}{2}, \frac{1}{2} \\
\frac{s+3}{2}, \left.\frac{s+3}{2} \right\rvert\,
\end{array} \right\rvert\, \frac{1}{4}\right)+\binom{s}{\frac{s}{2}}{ }_{3} F_{2}\left(\left.\begin{array}{c}
-\frac{s}{2},-\frac{s}{2},-\frac{s}{2} \\
1,-\frac{s-1}{2}
\end{array} \right\rvert\, \frac{1}{4}\right), \\
& \text { and } \\
& W_{4}(s)=\frac{\tan \left(\frac{\pi s}{2}\right)}{2^{2 s}}\binom{s}{\frac{s-1}{2}}^{3}{ }_{4} F_{3}\left(\left.\begin{array}{c}
\frac{1}{2}, \frac{1}{2}, \frac{1}{2}, \frac{s}{2}+1 \\
\frac{s+3}{2}, \frac{s+3}{2}, \left.\frac{s+3}{2} \right\rvert\,
\end{array} \right\rvert\, 1\right)+\binom{s}{\frac{s}{2}}{ }_{4} F_{3}\left(\left.\begin{array}{c}
\frac{1}{2},-\frac{s}{2},-\frac{s}{2},-\frac{s}{2} \\
1,1,-\frac{s-1}{2}
\end{array} \right\rvert\, 1\right) .
\end{aligned}
$$

## Simplifying the Meijer integrals for $W_{3}$ and $W_{4}$

- We (humans and/or computers) now obtained:


## Corollary (Hypergeometric forms for non-integer $s>-2$ )

$$
W_{3}(s)=\frac{\tan \left(\frac{\pi s}{2}\right)}{2^{2 s+1}}\binom{s}{\frac{s-1}{2}}^{2}{ }_{3} F_{2}\left(\left.\begin{array}{c}
\frac{1}{2}, \frac{1}{2}, \frac{1}{2} \\
\frac{s+3}{2}, \frac{s+3}{2}
\end{array} \right\rvert\, \frac{1}{4}\right)+\binom{s}{\frac{s}{2}}{ }_{3} F_{2}\left(\left.\begin{array}{c}
-\frac{s}{2},-\frac{s}{2},-\frac{s}{2} \\
1,-\frac{s-1}{2}
\end{array} \right\rvert\, \frac{1}{4}\right)
$$

and

$$
W_{4}(s)=\frac{\tan \left(\frac{\pi s}{2}\right)}{2^{2 s}}\binom{s}{\frac{s-1}{2}}^{3}{ }_{4} F_{3}\left(\left.\begin{array}{c}
\frac{1}{2}, \frac{1}{2}, \frac{1}{2}, \frac{s}{2}+1 \\
\frac{s+3}{2}, \frac{s+3}{2}, \frac{s+3}{2}
\end{array} \right\rvert\, 1\right)+\binom{s}{\frac{s}{2}} 4 F_{3}\left(\left.\begin{array}{c}
\frac{1}{2},-\frac{s}{2},-\frac{s}{2},-\frac{s}{2} \\
1,1,-\frac{s-1}{2}
\end{array} \right\rvert\, 1\right) .
$$

- We (humans) were able to provably take the limit at $\pm 1$ : e.g.,

$$
\begin{aligned}
W_{4}(-1) & =\frac{\pi}{4}{ }_{7} F_{6}\binom{\frac{5}{4}, \frac{1}{2}, \frac{1}{2}, \frac{1}{2}, \frac{1}{2}, \frac{1}{2}, \left.\frac{1}{2} \right\rvert\, 1}{\frac{1}{4}, 1,1,1,1,1}=\frac{\pi}{4} \sum_{n=0}^{\infty} \frac{(4 n+1)\binom{2 n}{n}^{6}}{4^{6 n}} \\
& =\frac{\pi}{4}{ }_{6} F_{5}\binom{\frac{1}{2}, \frac{1}{2}, \frac{1}{2}, \frac{1}{2}, \frac{1}{2}, \left.\frac{1}{2} \right\rvert\, 1}{1,1,1,1,1}+\frac{\pi}{64}{ }_{6} F_{5}\left(\left.\begin{array}{c}
\frac{3}{2}, \frac{3}{2}, \frac{3}{2}, \frac{3}{2}, \frac{3}{2}, \frac{3}{2} \\
2,2,2,2,2
\end{array} \right\rvert\, 1\right) .
\end{aligned}
$$

## Hypergeometric values of $W_{3}$ :

With much work involving moments of elliptic integrals we obtain:

## Theorem (Tractable hypergeometric form for $W_{3}$ )

(a) For $s \neq-3,-5,-7, \ldots$, we have

$$
W_{3}(s)=\frac{3^{s+3 / 2}}{2 \pi} \beta\left(s+\frac{1}{2}, s+\frac{1}{2}\right){ }_{3} F_{2}\left(\left.\begin{array}{c}
\frac{s+2}{2}, \frac{s+2}{2}, \frac{s+2}{2}  \tag{18}\\
1, \frac{s+3}{2}
\end{array} \right\rvert\, \frac{1}{4}\right) .
$$

(b) For every natural number $k=1,2, \ldots$,

$$
W_{3}(-2 k-1)=\frac{\sqrt{3}\binom{2 k}{k}^{2}}{2^{4 k+1} 3^{2 k}} 3 F_{2}\left(\left.\begin{array}{c}
\frac{1}{2}, \frac{1}{2}, \frac{1}{2} \\
k+1, k+1
\end{array} \right\rvert\, \frac{1}{4}\right) .
$$

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k+1, k+1
\end{array} \right\rvert\, \frac{1}{4}\right) .
$$

- The following formula hints at role played by Bessel functions (Kluywer 1906 and http:
//www.carma.newcastle.edu.au/jon/walks-anu.pdf):

$$
W_{n}=n \int_{0}^{\infty} J_{1}(x) J_{0}(x)^{n-1} \frac{\mathrm{dx}}{x} \approx \frac{\sqrt{n \pi}}{2} .
$$

## Contents

OPART I: Visual Theorems

- Visual theorems
- Large matrices
- Experimental mathematics


Digital Assistance

- Digital Assistance
- Simulation in Mathematics

3 PART II. Case Studies

- la. Iterated reflections
- lb: Protein conformation
- Ila: 100 digit challenge
- Ilb: Polylogarithms

PART III: Randomness

- Randomness is slippery
- Normality
- Normality of Pi
- BBP Digit Algorithms
- Some background
- Illa. Short rambles

6 Number walks

- Number walks (base four)

Walks on 'reals'

- IIIb: Study of number walks
- IIIc: Stoneham numbers
(3) Features of our walks
- Expected distance to origin
- Number of points visited
- Fractal and box-dimension


## Other realisations

- Fractals everywhere
- 3D drunkard's walks
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- 2-automatic numbers
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- References


## What is a (base four) random walk ?

Pick a random number in $\{0,1,2,3\}$ and move according to $0=\rightarrow, 1=\uparrow, 2=\leftarrow, 3=\downarrow$

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$$
1=\uparrow
$$

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$$
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Pick a random number in $\{0,1,2,3\}$ and move according to $0=\rightarrow, 1=\uparrow, 2=\leftarrow, 3=\downarrow$


$$
0=\rightarrow
$$

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Pick a random number in $\{0,1,2,3\}$ and move according to $0=\rightarrow, 1=\uparrow, 2=\leftarrow, 3=\downarrow$


## 11222330

## What is a random walk (base 4)?

Pick a random number in $\{0,1,2,3\}$ and move $0=\rightarrow, 1=\uparrow, 2=\leftarrow, 3=\downarrow$


Figure: A million step base-4 pseudorandom walk. We use the spectrum to show when we visited each point (ROYGBIV and R).

## Random walks look similarish



Figure: Eight different base-4 (pseudo)random ${ }^{8}$ walks of one million steps.

[^13]
## Base-b random walks:



Figure: Directions for base-3 and base-7 random walks.

## Contents

(1)
PART I: Visual Theorems

- Visual theorems
- Large matrices
- Experimental mathematics


Digital Assistance

- Digital Assistance
- Simulation in Mathematics
(3) PART II. Case Studies
- la. Iterated reflections
- lb: Protein conformation
- Ila: 100 digit challenge
- Ilb: Polylogarithms

PART III: Randomness

- Randomness is slippery
- Normality
- Normality of Pi
- BBP Digit Algorithms
- Some background
- Illa. Short rambles

Number walks

- Number walks (base four)
(7) Walks on 'reals'
- IIIb: Study of number walks
- IIIc: Stoneham numbers
(8) Features of our walks
- Expected distance to origin
- Number of points visited
- Fractal and box-dimension


## Other realisations

- Fractals everywhere
- 3D drunkard's walks
- Chaos games
- 2-automatic numbers
- Walks on the genome
- References


## III: Two rational numbers

## The base-4 digit expansion of $Q 1$ and $Q 2$ :

Q1=
0.221221012232121200122101223121001222100011232123121000122210001222 10001222100012221000012221000122201103010122010012010311033333333333 33333333333333330111111111111111111111111111100100000000300300320032 00320030223000322203000322230003022220300032223000322230003222300032 22320000232223000322230032221330023321233023213232112112121222323233 33303000001000323003230032203032030110333011103301103101111011332333 3232322321221211211121122322222122...

Q2 =
0.221221012232121200122101223121001222100011232123121000122210001222 10001222100012221000012221000122201103010122010012010311033333333333 33333333333333330111111111111111111111111111100100000000300300320032 00320030223000322203000322230003022220300032223000322230003222300032 22320000232223000322230032221330023321233023213232112112121222323233 33303000001000323003230032203032030110333011103301103101111011000000 000000 ...

## III: Two rational numbers



Figure: Self-referent walks on the rational numbers $Q 1$ (top) and $Q 2$ (bottom).

## Two more rationals

The following relatively small rational numbers [G. Marsaglia, 2010]

$$
Q 3=\frac{3624360069}{7000000001} \text { and } Q 4=\frac{123456789012}{1000000000061},
$$

have base-10 periods with huge length of 1,750,000,000 digits and $\mathbf{1 , 0 0 0 , 0 0 0 , 0 0 0 , 0 6 0}$ digits, respectively.

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have base-10 periods with huge length of 1,750,000,000 digits and $\mathbf{1 , 0 0 0 , 0 0 0 , 0 0 0 , 0 6 0}$ digits, respectively.


Figure: Walks on the first million base-10 digits of the rationals $Q 3$ and $Q 4$.

## Walks on the digits of numbers



Figure: A walk on the first 10 million base-4 digits of $\pi$.

## Walks on the digits of numbers

Coloured by hits (more pink is more hits)


Figure: 100 million base- 4 digits of $\pi$ coloured by number of returns to points.

## Contents

OPART I: Visual Theorems

- Visual theorems
- Large matrices
- Experimental mathematics


Digital Assistance

- Digital Assistance
- Simulation in Mathematics
(3) PART II. Case Studies
- la. Iterated reflections
- lb: Protein conformation
- Ila: 100 digit challenge
- Ilb: Polylogarithms

PART III: Randomness

- Randomness is slippery
- Normality
- Normality of Pi
- BBP Digit Algorithms
- Some background
- Illa. Short rambles


## Number walks

- Number walks (base four)
(7) Walks on 'reals'
- IIIb: Study of number walks
- IIIc: Stoneham numbers

8 Features of our walks

- Expected distance to origin
- Number of points visited
- Fractal and box-dimension

Other realisations

- Fractals everywhere
- 3D drunkard's walks
- Chaos games
- 2-automatic numbers
- Walks on the genome
- References


## The Stoneham numbers

$$
\alpha_{b, c}=\sum_{n=1}^{\infty} \frac{1}{c^{n} b^{n}}
$$

1973 Richard Stoneham proved some of the following (nearly 'natural') constants are $b$-normal for relatively prime integers $b, c$ :

$$
\alpha_{b, c}:=\frac{1}{c b^{c}}+\frac{1}{c^{2} b^{c^{2}}}+\frac{1}{c^{3} b^{c^{3}}}+\ldots
$$

Such super-geometric sums are Stoneham constants. To 10 places

$$
\alpha_{2,3}=\frac{1}{24}+\frac{1}{3608}+\frac{1}{3623878656}+\ldots
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Given coprime $b \geq 2$ and $c \geq 2$, such that $c<b^{c-1}$, the constant $\alpha_{b, c}$ is $b c$-nonnormal.

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Given coprime $b \geq 2$ and $c \geq 2$, such that $c<b^{c-1}$, the constant $\alpha_{b, c}$ is $b c$-nonnormal.

- Since $3<2^{3-1}=4, \alpha_{2,3}$ is 2-normal and 6-nonnormal !


## The Stoneham numbers

$$
\alpha_{b, c}=\sum_{n=1}^{\infty} \frac{1}{c^{n} b^{\pi} c^{\pi}}
$$



Figure: $\alpha_{2,3}$ is 2 -normal (top) but 6 -nonnormal (bottom). Is seeing believing?

## The Stoneham numbers

$$
\alpha_{b, c}=\sum_{n=1}^{\infty} \frac{1}{c^{n} b^{n}}
$$



Figure: Is $\alpha_{2,3}$ 3-normal or not?

## Contents

OPART I: Visual Theorems

- Visual theorems
- Large matrices
- Experimental mathematics


Digital Assistance

- Digital Assistance
- Simulation in Mathematics
 PART II. Case Studies
- la. Iterated reflections
- lb: Protein conformation
- Ila: 100 digit challenge
- Ilb: Polylogarithms

PART III: Randomness

- Randomness is slippery
- Normality
- Normality of Pi
- BBP Digit Algorithms
- Some background
- Illa. Short rambles

Number walks

- Number walks (base four)

Walks on 'reals'

- IIIb: Study of number walks
- IIIc: Stoneham numbers

8 Features of our walks

- Expected distance to origin
- Number of points visited
- Fractal and box-dimension

Other realisations

- Fractals everywhere
- 3D drunkard's walks
- Chaos games
- 2-automatic numbers
- Walks on the genome
- References


## The expected distance to the origin

Theorem
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$\left.\begin{array}{|c|c|c|c|c|}\hline \text { Number } & \text { Base } & \text { Steps } & \begin{array}{c}\text { Average normalized } \\ \text { dist. to the origin: } \\ \frac{1}{\text { Steps }} \sum_{N=2}^{\text {Steps }} \frac{\text { dist }}{N}\end{array} & \text { Normal } \frac{\sqrt{\pi N}}{2}\end{array}\right]$

## Contents

OPART I: Visual Theorems

- Visual theorems
- Large matrices
- Experimental mathematics


Digital Assistance

- Digital Assistance
- Simulation in Mathematics
(3) PART II. Case Studies
- la. Iterated reflections
- lb: Protein conformation
- Ila: 100 digit challenge
- Ilb: Polylogarithms

PART III: Randomness

- Randomness is slippery
- Normality
- Normality of Pi
- BBP Digit Algorithms
- Some background
- Illa. Short rambles

Number walks

- Number walks (base four)

Walks on 'reals'

- IIIb: Study of number walks
- IIIc: Stoneham numbers

8 Features of our walks

- Expected distance to origin
- Number of points visited
- Fractal and box-dimension
(9) Other realisations
- Fractals everywhere
- 3D drunkard's walks
- Chaos games
- 2-automatic numbers
- Walks on the genome
- References


## Number of points visited

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- 1988 D. Downham and S. Fotopoulos gave better bounds on the expectation. It lies in:

$$
\left(\frac{\pi(N+0.84)}{1.16 \pi-1-\log 2+\log (N+2)}, \frac{\pi(N+1)}{1.066 \pi-1-\log 2+\log (N+1)}\right) .
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$$

- For example, for $N=10^{6}$ these bounds are (199256.1,203059.5), while $\pi N / \log (N)=227396$, which overestimates the expectation.


## Catalan's constant

$$
G=1-1 / 4+1 / 9-1 / 16+\cdots
$$



Figure: A walk on one million quad-bits of $G$ with height showing frequency

## Paul Erdős (1913-1996)

## "My brain is open"


(a) Paul Erdős (Banff 1981. I was there)

(b) Émile Borel (1871-1956)

Figure: Two of my favourites. Consult MacTutor.

## Number of points visited:

## Again $\pi$ looks random


(a) (Pseudo)random walks.

(b) Walks built by chopping up 10 billion digits of $\pi$.

Figure: Number of points visited by 10,000 million-steps base- 4 walks.

## Points visited by various base-4 walks

| Number | Steps | Sites visited | Bounds on the expectation of sites visited by a random walk |  |
| :---: | :---: | :---: | :---: | :---: |
|  |  |  | Lower bound | Upper bound |
| Mean of 10,000 random walks | 1,000,000 | 202,684 | 199,256 | 203,060 |
| Mean of 10,000 walks on the digits of $\pi$ | 1,000,000 | 202,385 | 199,256 | 203,060 |
| $\alpha_{2,3}$ | 1,000,000 | 95,817 | 199,256 | 203,060 |
| $\alpha_{3,2}$ | 1,000,000 | 195,585 | 199,256 | 203,060 |
| $\pi$ | 1,000,000 | 204,148 | 199,256 | 203,060 |
| $\pi$ | 10,000,000 | 1,933,903 | 1,738,645 | 1,767,533 |
| $\pi$ | 100,000,000 | 16,109,429 | 15,421,296 | 15,648,132 |
| $\pi$ | 1,000,000,000 | 138,107,050 | 138,552,612 | 140,380,926 |
| $e$ | 1,000,000 | 176,350 | 199,256 | 203,060 |
| $\sqrt{2}$ | 1,000,000 | 200,733 | 199,256 | 203,060 |
| $\log 2$ | 1,000,000 | 214,508 | 199,256 | 203,060 |
| Champernowne $C_{4}$ | 1,000,000 | 548,746 | 199,256 | 203,060 |
| Rational number $Q_{1}$ | 1,000,000 | 378 | 199,256 | 203,060 |
| Rational number $Q_{2}$ | 1,000,000 | 939,322 | 199,256 | 203,060 |

## Normal numbers need not be so "random" ...



Figure: Champernowne $C_{10}=0.123456789101112 \ldots$ (normal). Normalized distance to the origin: 15.9 (50,000 steps).

## Normal numbers need not be so "random"



Figure: Champernowne $C_{4}=0.123101112132021 \ldots$ (normal). Normalized distance to the origin: 18.1 (100,000 steps). Points visited: 52760. Expectation: $(23333,23857)$.

## Normal numbers need not be so "random" ...



Figure: Stoneham $\alpha_{2,3}=0.0022232032 \ldots 4$ (normal base 4).
Normalized distance to the origin: 0.26 (1,000,000 steps).
Points visited: 95817. Expectation: $(199256,203060)$.

## Normal numbers need not be so "random" ...



Figure: Stoneham $\alpha_{2,3}=0.0022232032 \ldots 4$ (normal base 4).
Normalized distance to the origin: 0.26 (1,000,000 steps).
Points visited: 95817. Expectation: $(199256,203060)$.


Figure: A pattern in the digits of $\alpha_{2,3}$ base 4 . We show only positions of the walk after $\frac{3}{2}\left(3^{n}+1\right), \frac{3}{2}\left(3^{n}+1\right)+3^{n}$ and $\frac{3}{2}\left(3^{n}+1\right)+2 \cdot 3^{n}$ steps, $n=0,1, \ldots, 11$.

## Experimental conjecture

## Theorem (Base-4 structure of Stoneham $\alpha_{2,3}$ )

Denote by $a_{k}$ the $k^{\text {th }}$ digit of $\alpha_{2,3}$ in its base 4 expansion: $\alpha_{2,3}=\sum_{k=1}^{\infty} a_{k} / 4^{k}$, with $a_{k} \in\{0,1,2,3\}$ for all $k$. Then, for all $n=0,1,2, \ldots$ one has:
(i) $\sum_{k=\frac{3}{2}\left(3^{n}+1\right)}^{\frac{3}{2}\left(3^{n}+1\right)+3^{n}} e^{a_{k} \pi i / 2}=\left\{\begin{array}{lc}-i, & n \text { odd } \\ -1, & \mathrm{n} \text { even }\end{array}\right.$;
(ii) $a_{k}=a_{k+3^{n}}=a_{k+2 \cdot 3^{n}}$ if $k=\frac{3\left(3^{n}+1\right)}{2}, \frac{3\left(3^{n}+1\right)}{2}+1, \ldots, \frac{3\left(3^{n}+1\right)}{2}+3^{n}-1$.


## Likewise, $\alpha_{3,5}$ is 3 -normal ... but not very "random" ANIMATION

## Contents

OPART I: Visual Theorems

- Visual theorems
- Large matrices
- Experimental mathematics


Digital Assistance

- Digital Assistance
- Simulation in Mathematics
(3) PART II. Case Studies
- la. Iterated reflections
- lb: Protein conformation
- Ila: 100 digit challenge
- Ilb: Polylogarithms

PART III: Randomness

- Randomness is slippery
- Normality
- Normality of Pi
- BBP Digit Algorithms
- Some background
- Illa. Short rambles

Number walks

- Number walks (base four)

Walks on 'reals'

- IIIb: Study of number walks
- IIIc: Stoneham numbers

8 Features of our walks

- Expected distance to origin
- Number of points visited
- Fractal and box-dimension
(9) Other realisations
- Fractals everywhere
- 3D drunkard's walks
- Chaos games
- 2-automatic numbers
- Walks on the genome
- References


## Box-dimension:



$$
\text { Box-dimension }=\lim _{\text {side } \rightarrow 0} \frac{\log (\# \text { boxes })}{\log (1 / \text { side })}
$$

Norway is "frillier" - Hitchhiker's Guide to the Galaxy

## Box-dimension:

## Tends to '2' for a planar random walk



Fractals: self-similar (zoom invariant) partly space-filling shapes (clouds \& ferns not buildings \& cars). Curves have dimension 1 , squares dimension 2

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## Contents

OPART I: Visual Theorems

- Visual theorems
- Large matrices
- Experimental mathematics


Digital Assistance

- Digital Assistance
- Simulation in Mathematics
(3) PART II. Case Studies
- la. Iterated reflections
- lb: Protein conformation
- Ila: 100 digit challenge
- Ilb: Polylogarithms

PART III: Randomness

- Randomness is slippery
- Normality
- Normality of Pi
- BBP Digit Algorithms
- Some background
- Illa. Short rambles

Number walks

- Number walks (base four)


## Walks on 'reals'

- IIIb: Study of number walks
- IIIc: Stoneham numbers

Features of our walks

- Expected distance to origin
- Number of points visited
- Fractal and box-dimension

9 Other realisations

- Fractals everywhere
- 3D drunkard's walks
- Chaos games
- 2-automatic numbers
- Walks on the genome
- References


## Fractals everywhere

## From Mars



## Fractals everywhere

## From Mars •sor



The picture fractalized by the Barnsley's
http://frangostudio.com/frangocamera.html

## Fractals everywhere

## From Space



## Fractals everywhere



## Fractals everywhere



## Fractals everywhere



## Fractals everywhere



Pascal triangle modulo two $[1][1,1][1,2,1][1,3,3,1],[1,4,6,4,1][1,510,10,5,1] \ldots$

## Fractals everywhere



Steps to construction of a Sierpinski cube

## Fractals everywhere

## The Sierpinski Triangle

$$
1 \mapsto 3 \mapsto 9
$$



## Fractals everywhere

## The Sierpinski Triangle

$$
1 \mapsto 3 \mapsto 9
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## Fractals everywhere

## The Sierpinski Triangle

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## Fractals everywhere

## The Sierpinski Triangle

$$
1 \mapsto 3 \mapsto 9
$$



http:
//oldweb.cecm.sfu.ca/cgi-bin/organics/pascalform

## Contents

(1)PART I: Visual Theorems

- Visual theorems
- Large matrices
- Experimental mathematics


Digital Assistance

- Digital Assistance
- Simulation in Mathematics

3 PART II. Case Studies

- la. Iterated reflections
- lb: Protein conformation
- Ila: 100 digit challenge
- Ilb: Polylogarithms
- Randomness is slippery
- Normality
- Normality of Pi
- BBP Digit Algorithms
- Some background
- Illa. Short rambles

Number walks

- Number walks (base four)


## Walks on 'reals'

- IIIb: Study of number walks
- IIIc: Stoneham numbers

Features of our walks

- Expected distance to origin
- Number of points visited
- Fractal and box-dimension
(9) Other realisations
- Fractals everywhere
- 3D drunkard's walks
- Chaos games
- 2-automatic numbers
- Walks on the genome
- References


## Three dimensional walks:



Figure: Matt Skerritt's 3D walk on $\pi$ (base 6), showing one million steps. But 3D random walks are not recurrent.

## Three dimensional walks:



Figure: Matt Skerritt's 3D walk on $\pi$ (base 6), showing one million steps. But 3D random walks are not recurrent.
"A drunken man will find his way home, a drunken bird will get lost forever." (Kakutani)

## Three dimensional printing:



Figure: The future is here ...
www.digitaltrends.com/cool-tech/the-worlds-first-plane-created-entirely-by-3d-printing-takes-flight/
www.shapeways.com/shops/3Dfractals

## Contents

OPART I: Visual Theorems

- Visual theorems
- Large matrices
- Experimental mathematics


Digital Assistance

- Digital Assistance
- Simulation in Mathematics

3 PART II. Case Studies

- la. Iterated reflections
- lb: Protein conformation
- Ila: 100 digit challenge
- Ilb: Polylogarithms

PART III: Randomness

- Randomness is slippery
- Normality
- Normality of Pi
- BBP Digit Algorithms
- Some background
- Illa. Short rambles

Number walks

- Number walks (base four)


## Walks on 'reals'

- IIIb: Study of number walks
- IIIc: Stoneham numbers

Features of our walks

- Expected distance to origin
- Number of points visited
- Fractal and box-dimension
(9) Other realisations
- Fractals everywhere
- 3D drunkard's walks
- Chaos games
- 2-automatic numbers
- Walks on the genome
- References


## Chaos games:



Figure: Coloured by frequency - leads to random fractals. Row 1: Champernowne $C_{3}, \alpha_{3,5}$, random, $\alpha_{2,3}$. Row 2: Champernowne $C_{4}$, $\pi$, random, $\alpha_{2,3}$. Row 3: Champernowne $C_{6}, \alpha_{3,2}$, random, $\alpha_{2,3}$.

## Contents

PART I: Visual Theorems

- Visual theorems
- Large matrices
- Experimental mathematics


Digital Assistance

- Digital Assistance
- Simulation in Mathematics

3 PART II. Case Studies

- la. Iterated reflections
- lb: Protein conformation
- Ila: 100 digit challenge
- Ilb: Polylogarithms
- Randomness is slippery
- Normality
- Normality of Pi
- BBP Digit Algorithms
- Some background
- Illa. Short rambles


## Number walks

- Number walks (base four)


## Walks on 'reals'

- IIIb: Study of number walks
- IIIc: Stoneham numbers

Features of our walks

- Expected distance to origin
- Number of points visited
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(9) Other realisations
- Fractals everywhere
- 3D drunkard's walks
- Chaos games
- 2-automatic numbers
- Walks on the genome
- References


## Automatic numbers: Thue-Morse and Paper-folding

Automatic numbers are never normal. They are given by simple but fascinating rules...giving structured/boring walks:


Figure: Paper folding. The sequence of left and right folds along a strip of paper that is folded repeatedly in half in the same direction. Unfold and read 'right' as ' 1 ' and 'left' as ' 0 ': 10110011100100

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Thue-Morse constant (transcendental; 2-automatic, hence nonnormal):

$$
\begin{gathered}
T M_{2}=\sum_{n=1}^{\infty} \frac{1}{2^{t(n)}} \text { where } t(0)=0, \text { while } t(2 n)=t(n) \text { and } t(2 n+1)=1-t(n) \\
0.01101001100101101001011001101001 \ldots
\end{gathered}
$$

## Automatic numbers: Thue-Morse and Paper-folding

Automatic numbers are never normal. They are given by simple but fascinating rules...giving structured/boring walks:

(a) 1,000 bits of Thue-Morse sequence.
(b) 10 million bits of paperfolding sequence.

Figure: Walks on two automatic and so nonnormal numbers.

## Automatic numbers: <br> Turtle plots look great!


(a) Ten million digits of the paperfolding sequence, rotating $60^{\circ}$.

(c) 100,000 digits of the ThueMorse sequence, rotating $60^{\circ}$ (a Koch snowflake).
(b) One million digits of the paperfolding sequence, rotating $120^{\circ}$ (a dragon curve).

(d) One million digits of $\pi$, rotating $60^{\circ}$.

Figure: Turtle plots on various constants with different rotating angles in base 2 -where ' $\mathbf{0}$ ' yields forward motion and ' 1 ' rotation by a fixed angle.

## Contents

OPART I: Visual Theorems

- Visual theorems
- Large matrices
- Experimental mathematics

Digital Assistance

- Digital Assistance
- Simulation in Mathematics
(3) PART II. Case Studies
- la. Iterated reflections
- lb: Protein conformation
- Ila: 100 digit challenge
- Ilb: Polylogarithms
- Randomness is slippery
- Normality
- Normality of Pi
- BBP Digit Algorithms
- Some background
- Illa. Short rambles

Number walks

- Number walks (base four)

Walks on 'reals'

- IIIb: Study of number walks
- IIIc: Stoneham numbers

Features of our walks

- Expected distance to origin
- Number of points visited
- Fractal and box-dimension
(9) Other realisations
- Fractals everywhere
- 3D drunkard's walks
- Chaos games
- 2-automatic numbers
- Walks on the genome
- References


## Genomes as walks:

We are all base 4 numbers (ACGT/U)

Chromosome X

$$
\begin{aligned}
c & =[1,0] \\
g & =[0,1] \\
t & =[-1,0] \\
a & =[0,-1]
\end{aligned}
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The X Chromosome (34K) and Chromosome One (10K).

## Genomes as walks:

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$$



The X Chromosome (34K) and Chromosome One (10K).
® Chromosomes look less like $\pi$ and more like concatenation numbers?

## DNA for Storage:

News Science $\rangle$ Biochemistry and molecular biology
Shakespeare and Martin Luther King demonstrate potential of DNA storage All 154 Shakespeare sonnets have been spelled out in DNA to demonstrate the vast potential of genetic data storage
lan Sample, science correspondent
The Guardian, Thursday 24 January 2013
Jump to comments (...)


When written in DNA, one of Shakespeare's sonnets weighs 0.3 millionths of a millionth of a gram. Photograph: Oli Scarff/Getty


Figure: The potential for DNA storage ( L ) and the quadruple helix ( R )

## The end

## with some fractal dessert



## with some fractal dessert



## Thank you

## Contents

OPART I: Visual Theorems

- Visual theorems
- Large matrices
- Experimental mathematics


Digital Assistance

- Digital Assistance
- Simulation in Mathematics
(3) PART II. Case Studies
- la. Iterated reflections
- lb: Protein conformation
- Ila: 100 digit challenge
- Ilb: Polylogarithms
- Randomness is slippery
- Normality
- Normality of Pi
- BBP Digit Algorithms
- Some background
- Illa. Short rambles

Number walks

- Number walks (base four)


## Walks on 'reals'

- IIIb: Study of number walks
- IIIc: Stoneham numbers

Features of our walks

- Expected distance to origin
- Number of points visited
- Fractal and box-dimension
(9) Other realisations
- Fractals everywhere
- 3D drunkard's walks
- Chaos games
- 2-automatic numbers
- Walks on the genome
- References
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[^0]:    ${ }^{1}$ J.E. Littlewood, A mathematician's miscellany, London: Methuen (1953); Littlewood, J. E. and Bollobás, Béla, ed., Littlewood's miscellany, Cambridge University Press, 1986.

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[^2]:    ${ }^{2}$ See http://www.carma.newcastle.edu.au/jon/Completion.pdf and http://www.carma.newcastle.edu.au/jon/dr-fields11.pptx.

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[^4]:    ${ }^{2}$ See http://www. carma.newcastle.edu.au/jon/Completion.pdf and http://www.carma.newcastle.edu.au/jon/dr-fields11.pptx.

[^5]:    In Adrian Rice, "What Makes a Great Mathematics Teacher?" MAA Monthly, 1999.

[^6]:    ${ }^{3} \mathrm{~A}$ cross-section of such resources is available through
    http://www.carma.newcastle.edu.au/jon/portal.html and www.experimentalmath.info.

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[^8]:    ${ }^{4}$ RuBisCO (responsible for photosynthesis) has 550 amino acids (smallish).
    ${ }^{5} \mathrm{~A}$ coupling which occurs through space, rather than chemical bonds.

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[^10]:    ${ }^{4}$ RuBisCO (responsible for photosynthesis) has 550 amino acids (smallish).
    ${ }^{5} \mathrm{~A}$ coupling which occurs through space, rather than chemical bonds.

[^11]:    ${ }^{6}$ Only the best get stamps. Quoted in
    www-history.mcs.st-andrews.ac.uk/Quotations/Banach.html.

[^12]:    ${ }^{7}$ Quadrature was our first interest

[^13]:    

