Short Walks and Ramble Integrals: the Arithmetic of Uniform Random Walks

54th Annual AustMS Meeting

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Joint with Dirk Nuyens, Armin Straub, James Wan & Wadim Zudilin

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Director, CARMA, the University of Newcastle

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Outline

1. Introduction
2. Combinatorics
3. Analysis
4. Probability
5. Open Problems

I. INTRODUCTION

- An age old question: What is a walk?

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- An age old question: What is a walk?
- Also random walks, random migrations, random flights.

Abstract

Following Pearson in **1905**, we study the expected distance of a two-dimensional walk in the plane with n unit steps in random directions — what Pearson called a random walk or a "ramble".

> *While the statistics and large n behaviour are well understood, the precise behaviour of the first few steps is quite remarkable and less tractable.*

Series evaluations and recursions are obtained making it possible to explicitly determine this distance for small number of steps. Hypergeometric and elliptic *hyper-closed*[1] form expressions are given for the densities and all the moments of a 2, 3 or 4-step walk.

Heavy use is made of analytic continuation of the integral (also of modern special functions and computer algebra (CAS)).

[1] JMB & Crandall, "Closed forms: what they are and why they matter," *Notices of the AMS*, in press. See `http://www.carma.newcastle.edu.au/~jb616/closed-form.pdf`

"**Birds and Frogs**" (Freeman Dyson, *NAMS* 2010)

Some mathematicians are birds, others are frogs. Birds fly high in the air and survey broad vistas of mathematics out to the far horizon. They delight in concepts that unify our thinking and bring together diverse problems from different parts of the landscape. Frogs live in the mud below and see only the flowers that grow nearby. They delight in the details of particular objects, and they solve problems one at a time.

I happen to be a frog, but many of my best friends are birds. The main theme of my talk tonight is this. Mathematics needs both birds and frogs. Mathematics is rich and beautiful because birds give it broad visions and frogs give it intricate details.

Mathematics is both great art and important science, because it combines generality of concepts with depth of structures. It is stupid to claim that birds are better than frogs because they see farther, or that frogs are better than birds because they see deeper.

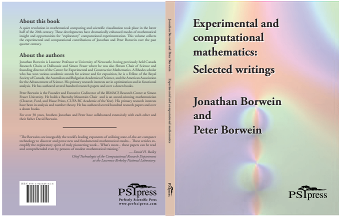
...

"Experimental and Computational Mathematics"

Discussion. This article[2] is one of our favourites.

Mathematics has frequently seen alternating periods of theory building and periods of pathology hunting. The first without the second leads to sterile structures save for a few Grothendiecks. The second without the first runs out of steam and one is left only with something akin to a pre-Linnaean taxonomy in which no structures are to be discerned.

PsiPress iBook, 2010



In his wonderful *Notices* article Birds and Frogs Freeman Dyson makes the same point forcibly and elegantly. In Dyson's terms we are unabashed frogs who consume the droppings of friendly birds thereby enriching the pond's nutrients for future visiting birds.

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[2] "*Strange series evaluations and high precision fraud*," *MAA Monthly*, 1992.

Exploratory Experimentation and Computation in Mathematics: ... and so to have 'Fun'

- Numbers, symbols, and pictures let us explore, refute and refine conjectures (throughout this work).
- Even to obtain secure knowledge in areas where formal proof is out of reach. See:
  - Presentation: www.carma.newcastle.edu.au/~jb616/expexp10.ppsx
  - Extended paper: www.carma.newcastle.edu.au/~jb616/expexp.pdf (*Notices*, in press, with Bailey)

Random walk integrals — our starting point

For complex s

Definition

$$W_n(s) := \int_{[0,1]^n} \left| \sum_{k=1}^n e^{2\pi x_k i} \right|^s \mathrm{d}\boldsymbol{x}$$

- W_n is analytic precisely for $\Re s > -2$.
- Also, let $W_n := W_n(1)$ denote the *expectation*.

Simplest case (obvious for geometric reasons):

$$W_1(s) = \int_0^1 \left| e^{2\pi i x} \right|^s \mathrm{d}x = 1.$$

- 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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- There is always a 1-dimension reduction

$$\begin{aligned} W_n(s) &= \int_{[0,1]^n} \left| \sum_{k=1}^{n} e^{2\pi x_k i} \right|^s \mathrm{d}\boldsymbol{x} \\ &= \int_{[0,1]^{n-1}} \left| 1 + \sum_{k=1}^{n-1} e^{2\pi x_k i} \right|^s \mathrm{d}(x_1, \ldots, x_{n-1}) \end{aligned}$$

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- So $W_2 = 4\int_0^{1/2} \cos(\pi x)\mathrm{d}x \ = \ \frac{4}{\pi}$.

$n \geq 3$ highly nontrivial and $n \geq 5$ still not well understood.

- Similar problems often get *much* more difficult in five dimensions and above — e.g., Bessel moments, Box integrals, Ising integrals (work with Bailey, Broadhurst, Crandall, ...).

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- We have a general program to develop symbolic numeric techniques for multi-dim integrals (as illustrated in JW's talk).

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When the facts change, I change my mind. What do you do, sir?
— John Maynard Keynes in *Economist* Dec 18, 1999.

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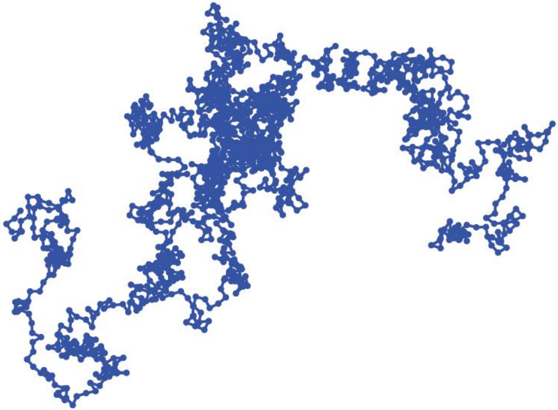
One 1500-step ramble: a familiar picture



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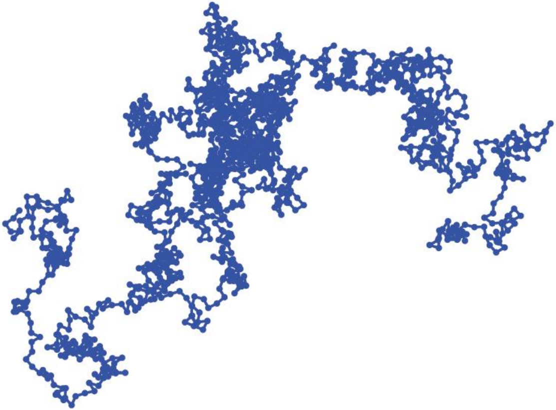

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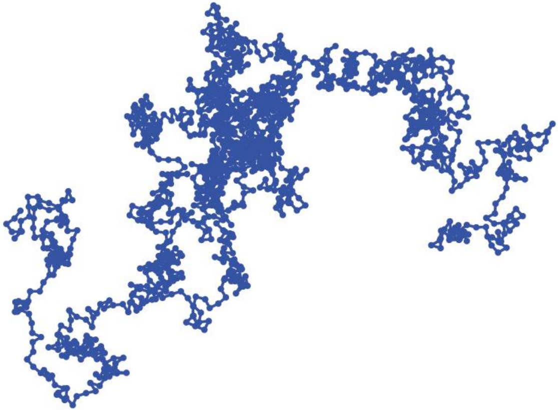
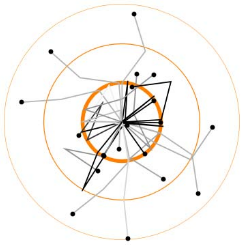


- 1D (and 3D) easy. Expectation of RMS distance is easy ($\sqrt{n}$).
- 1D or 2D *lattice*: probability one of returning to the origin.

1000 three-step rambles: a less familiar picture?



A little history — from a vast literature

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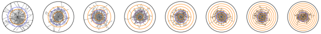
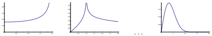
- **UNSW**: Donovan and Nuyens, WWII cryptography.
- Appear in quantum chemistry, in quantum physics as hexagonal and diamond lattice integers, etc ...

Armin Straub's Tulane Poster

Random Walk Integrals

Armin Straub. Joint work with Jonathan M. Borwein, Dirk Nuyens, James Wan
Mathematics Department, Tulane University





Introduction

- We study random walks in the plane consisting of n steps. Each step is of length 1 and is taken in a randomly chosen direction.

- We are interested in the distance traveled in n steps. For instance, how large is this distance on average?
- Represent the kth step by the complex number $e^{2\pi i x_k}$. Then we see that the sth moment of the distance after n steps is:

$$W_n(s) := \int_{[0,1]^n} \left| \sum_{k=1}^n e^{2\pi x_k i} \right|^s \mathrm{d}\boldsymbol{x} \qquad (1)$$

In particular, $W_n(1)$ is the average distance after n steps.
- (1) is hard to evaluate numerically to high precision. For instance, Monte-Carlo integration gives approximations with an asymptotic error of $O(1/\sqrt{N})$ where N is the number of sample points.

History and applications

- Considered in 1880 by Lord Rayleigh in the composition of n vibrations with same frequency and random phase.
- Used in 1904 by Ronald Ross to model the dispersion of mosquitoes.
- Further studied by Karl Pearson, J. C. Kluyver, and many others; particularly successful, for instance, in the context of random migration of micro-organisms or the phenomenon of laser speckle.
- While W_n is well understood for large n, there is still much interest in the case of small n.

Explicit evaluations

- $W_1(s) = 1$.
- $W_2(s) = \binom{s}{s/2}$. In particular, $W_2(1) = \frac{4}{\pi} \approx 1.27324$.
- For integers k we have

$$W_3(k) = \operatorname{Re}\ {}_3F_2\left(\left. \begin{matrix} \frac{1}{2}, -\frac{k}{2}, -\frac{k}{2} \\ 1, 1 \end{matrix} \right| 4 \right). \qquad (2)$$

In particular, $W_3(1) = \frac{3}{16} \cdot \frac{2^{1/3}}{\pi^4} \Gamma^6\left(\frac{1}{3}\right) + \frac{27}{4} \cdot \frac{2^{2/3}}{\pi^4} \Gamma^6\left(\frac{2}{3}\right) \approx 1.57460.$

From Analysis to Combinatorics ...

- For even $s = 2k$ we get integers!

$$W_n(2k) =: f_n(k) = \sum_{a_1+\cdots+a_n=k} \binom{k}{a_1, \ldots, a_n}^2. \qquad (3)$$

- $f_n(k)$ counts the number of *abelian squares*: strings xy of length $2k$ from an alphabet with n letters such that y is a permutation of x.
- For instance, *acbc ccba* contributes to $f_3(4)$.
- Surely: $f_1(k) = 1$.
- Just a bit harder: $f_2(k) = \binom{2k}{k}$ which can be seen from
  $b\,\underline{a}\,b\,\underline{a}\,\underline{a}$ $\;a\,\underline{b}\,a\,a\,\underline{b}$.
- Summation formulae for $n > 2$ can be obtained from the convolution

$$f_{n+m}(k) = \sum_{j=0}^k \binom{k}{j}^2 f_n(j) f_m(k-j). \qquad (4)$$

- The machinery of combinatorics ensures recurrences for fixed n. For instance, for $n = 4$:
$(k+2)^3 f_4(k+2) - 2(2k+3)(5k^2+15k+12) f_4(k+1) + 64(k+1)^3 f_4(k) = 0$

... and back to Analysis

- Via Carlson's Theorem the combinatorial recurrences can be lifted to functional equations. For instance:
$(s+4)^3 W_4(s+4) - 4(s+3)(5s^2+30s+48) W_4(s+2) + 64(s+2)^3 W_4(s) = 0$
- It follows that $W_n(s)$ is a meromorphic function in s with poles at certain negative integers.
- From (3), we have the following generating function:

$$\sum_{k\geqslant 0} W_n(2k) \frac{(-x)^k}{(k!)^2} = \left(\sum_{k\geqslant 0} \frac{(-x)^k}{(k!)^2} \right)^n = J_0(2\sqrt{x})^n$$

where $J_n(z)$ denotes the Bessel function of the first kind. Applying Ramanujan's master theorem we are led to

$$W_n(-s) = 2^{1-s} \frac{\Gamma(1-s/2)}{\Gamma(s/2)} \int_0^\infty x^{s-1} J_0^n(x)\, \mathrm{d}x. \qquad (5)$$

- Formula (5), which was found by David Broadhurst, is quite suitable for high precision evaluations.

Further study

- Inspired by (4), we conjecture that for complex s

$$W_{2n}(s) \stackrel{?}{=} \sum_{j\geqslant 0} \binom{s/2}{j}^2 W_{2n-1}(s-2j).$$

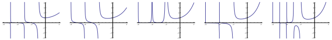
- Coupled with (2) this gives a very efficient method to evaluate $W_4(k)$ to high precision. What about $W_5(k)$?

Reference:
J. Borwein, D. Nuyens, A. Straub, and J. Wan. *"Random walk integrals."* submitted, March 2010.

This work was supported by an IBM Fellowship in Computational Science.

n	$s=1$	$s=3$	$s=5$	$s=7$	$s=9$
2	1.27324	3.39531	10.8650	37.2514	132.449
3	1.57460	6.45168	36.7052	241.544	1714.62
4	1.79909	10.1207	82.6515	822.273	9169.62
5	2.00816	14.2896	152.316	2037.14	31393.1
6	2.19386	18.9133	248.759	4186.19	82718.9

n	$s=2$	$s=4$	$s=6$	$s=8$	$s=10$	Sloane's
2	2	6	20	70	252	A000984
3	3	15	93	639	4653	A002893
4	4	28	256	2716	31504	A002895
5	5	45	545	7885	127905	
6	6	66	996	18306	384156	



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James Wan's Three Minute Thesis

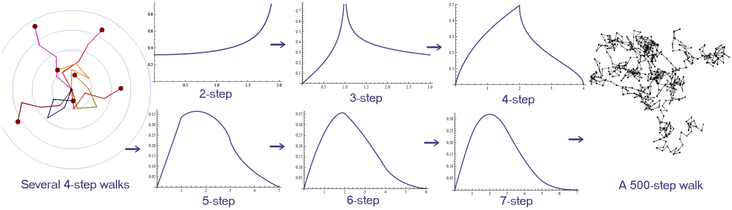
Computer Assisted Mathematical Analysis and Number Theory

James Wan

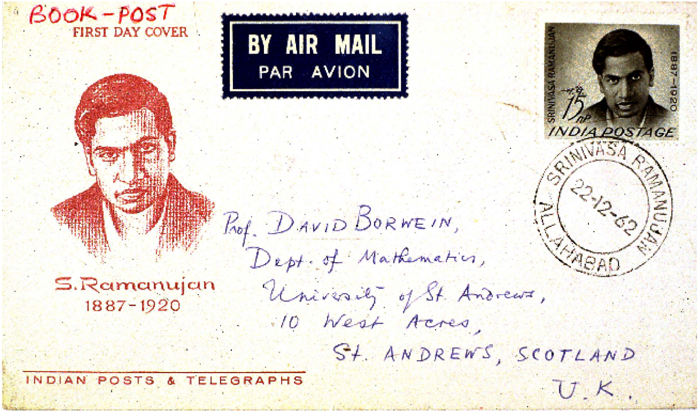
Example (Random Walks)

Take n steps on a flat surface, each of length 1 and chosen in a random direction. What is the average distance to the starting position?

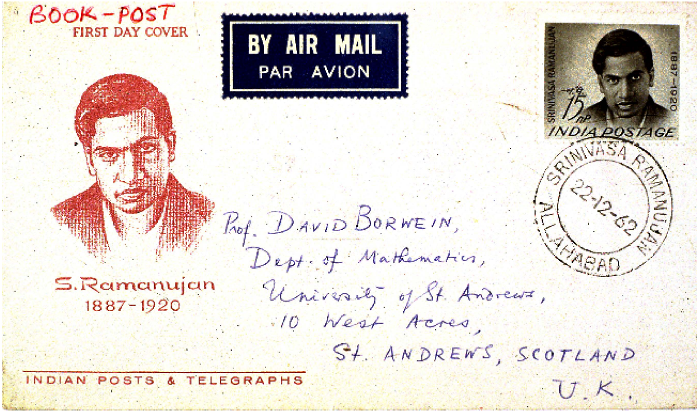
- We recast the problem as a *high dimensional integral*.
- 2-step average $= \frac{4}{\pi}$. 3-step average $= \frac{16\sqrt[3]{4}\pi^2}{\Gamma(\frac{1}{3})^6} + \frac{3\Gamma(\frac{1}{3})^6}{8\sqrt[3]{4}\pi^4} \approx 1.574597$



II. COMBINATORICS



II. COMBINATORICS



- I am planning a 2012 celebration when my favourite frog turns $125 = 5^3 = 11^2 + 2^2 = 10^2 + 5^2 = 15^2 - 10^2 = \ldots$.

$W_n(k)$ at even values

Even values are easier (combinatorial – no square roots).

k	0	2	4	6	8	10
$W_2(k)$	1	2	6	20	70	252
$W_3(k)$	1	3	15	93	639	4653
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$W_5(k)$	1	5	45	545	**7885**	**127905**

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- *MathWorld* gives $W_n(2) = n$ (trivial).

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- Observe that $W_2(s) = \binom{s}{s/2}$ for $s > -1$.
- *MathWorld* gives $W_n(2) = n$ (trivial).
- Entering 1,5,45,545 in the *OIES* now gives *"The function $W_5(2n)$ (see Borwein et al. reference for definition)."*

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Memorize this number!

During the three years which I spent at Cambridge my time was wasted, as far as the academical studies were concerned, as completely as at Edinburgh and at school. I attempted mathematics, and even went during the summer of 1828 with a private tutor (a very dull man) to Barmouth, but I got on very slowly. The work was repugnant to me, chiefly from my not being able to see any meaning in the early steps in algebra. This impatience was very foolish, and in after years I have deeply regretted that I did not proceed far enough at least to understand something of the great leading principles of mathematics, for men thus endowed seem to have an extra sense. — Autobiography of Charles Darwin

Resolution at even values

- Even formula counts n-letter abelian squares $x\pi(x)$ of length $2k$ (Shallit-Richmond (2008) give asymptotics):

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- Known to satisfy convolutions:

$$W_{n_1+n_2}(2k) = \sum_{j=0}^{k} \binom{k}{j}^2 W_{n_1}(2j) W_{n_2}(2(k-j)), \text{ so}$$

$$W_5(2k) = \sum_j \binom{k}{j}^2 \binom{2(k-j)}{k-j} \sum_\ell \binom{j}{\ell}^2 \binom{2\ell}{\ell} = \sum_j \binom{k}{j}^2 \sum_\ell \binom{2(j-\ell)}{j-\ell} \binom{j}{\ell}^2 \binom{2\ell}{\ell}$$

Resolution at even values

- Even formula counts n-letter abelian squares $x\pi(x)$ of length $2k$ (Shallit-Richmond (2008) give asymptotics):

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$$W_{n_1+n_2}(2k) = \sum_{j=0}^{k} \binom{k}{j}^2 W_{n_1}(2j) W_{n_2}(2(k-j)), \text{ so}$$

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- and recursions such as:

$$(k+2)^2 W_3(2k+4) - (10k^2+30k+23) W_3(2k+2) + 9(k+1)^2 W_3(2k) = 0.$$

A binomial expansion of $W_n(s)$

- Recall $W_n(s) := \int_{[0,1]^n} \left| \sum_{k=1}^{n} e^{2\pi x_k i} \right|^s \mathrm{d}\boldsymbol{x}$.

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- Experimentally we found recursion for $I_{3,m} \ldots$

Our conjectural route ...

- Looked up $I_{3,m}$ on Sloane's **OEIS** (as on next slide) get

$$\underline{1, 6, 42, 312, 2394}, 18756, 149136, \ldots$$

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OEIS at work, see `www.research.att.com/~njas/sequences`.

AT&T Integer Sequences RESEARCH

Greetings from The On-Line Encyclopedia of Integer Sequences!

1,6,42,312,2394 [Search] Hints

Search: **1, 6, 42, 312, 2394**

Displaying 1-1 of 1 results found. page 1

Format: long | short | internal | text Sort: relevance | references | number Highlight: on | off

A093388 (n+1)^2 a_{n+1} = (17n^2+17n+6) a_n - 72n^2 a_{n-1}. +20 1

1, 6, 42, 312, 2394, 18756, 149136, 1199232, 9729882, 79527084, 654089292, 5408896752, 44941609584, 375002110944, 3141107339328, 26402533581312, 222635989516122, 1882882811380284, 15967419789558804, 135752058036988848, 1156869080242393644 (list; graph; listen)

OFFSET	0,2
COMMENT	This is the Taylor expansion of a special point on a curve described by Beauville.
REFERENCES	Arnaud Beauville, Les familles stables de courbes sur P_1 admettant quatre fibres singulieres, Comptes Rendus, Academie Science Paris, no. 294, May 24 1982. Matthijs Coster, Over 6 families van krommen [On 6 families of curves], Master's Thesis (unpublished), Aug 26 1983.
LINKS	Matthijs Coster, Sequences H. Verrill, Some congruences related to modular forms, Section 2.2.
FORMULA	(-1)^n * sum_{k=0}^n binomial(n, k) * (-8)^k * sum_{j=0}^{n-k} binomial(n-k, j)^3 - Helena Verrill (verrill(AT)math.lsu.edu), Aug 09 2004
MAPLE	f:=proc(n) option remember; local m; if n=0 then RETURN(1); fi; if n=1 then RETURN(6); fi; m:=n-1; ((17*m^2+17*m+6)*f(n-1)-72*m^2*f(n-2))/n^2; end;
PROGRAM	(PARI) a(n)=(-1)^n*sum(k=0, n, binomial(n, k)*(-8)^k*sum(j=0, n-k, binomial(n-k, j)^3))
CROSSREFS	This is the seventh sequence in the family beginning A002894, A006077, A081085, A005258, A000172, A002893. Sequence in context: A111602 A091164 A004982 this_sequence A162968 A034171 A153293 Adjacent sequences: A093385 A093386 A093387 this_sequence A093389 A093390 A093391
KEYWORD	nonn
AUTHOR	Matthijs Coster (matthijs(AT)coster.demon.nl), Apr 29 2004

page 1

Search completed in 0.003 seconds

. . . and proof

- Needed to show

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is the constant term of

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- To preserve symmetry, we did not use the dimension reduction.
- Now expanded the m-th power on both sides, and amazingly corresponding terms are equal. So (2) holds. **QED**

- So W_n satisfies an $\lfloor \frac{n+1}{2} \rfloor$-term recursion and can be given by $\lfloor \frac{n+3}{2} \rfloor$ distinct iterated sums:
  For instance

$$
\begin{aligned}
W_3 &= 3\sum_{n=0}^{\infty}\binom{1/2}{n}\left(-\frac{8}{9}\right)^n \sum_{k=0}^{n}\binom{n}{k}\left(-\frac{1}{8}\right)^k \sum_{j=0}^{k}\binom{k}{j}^3 \\
&= 3\sum_{n=0}^{\infty}(-1)^n\binom{1/2}{n}\sum_{k=0}^{n}\binom{n}{k}\left(-\frac{1}{9}\right)^k \sum_{j=0}^{k}\binom{k}{j}^2\binom{2j}{j}
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- Tanh-sinh (doubly-exponential) quadrature works well for W_3 but not so well for $W_4 \approx 1.79909248$.
- Quasi-Monte Carlo was *not* very accurate (JW's prior talk).

Binomial Transform

Theorem (binomial involution)

Given real sequences (a_n) *and* (s_n), *the following are equivalent:*

$$s_n = \sum_{k=0}^{n} (-1)^k \binom{n}{k} a_k,$$

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We can now give a **proof** of the even formula (1). Apply

$$W_n(2j) = n^{2i} \sum_{m \geqslant 0} (-1)^m \binom{\frac{2j}{2}}{m} \sum_{k=0}^{m} \frac{(-1)^k}{n^{2k}} \binom{m}{k} \sum_{\sum a_i = k} \binom{k}{a_1, \ldots, a_n}^2,$$

and appeal to the involution. **QED**

III. ANALYSIS

   

   

Midtalk test: Who are we? Answers later!

Carlson's theorem: from discrete to continuous

Theorem (Carlson (1914, PhD))

If $f(z)$ is analytic for $\Re(z) \geq 0$, its growth on the imaginary axis is bounded by $e^{cy}, |c| < \pi$, and

$$0 = f(0) = f(1) = f(2) = \ldots$$

then $f(z) = 0$ identically.

- $\sin(\pi z)$ does not satisfy the conditions of the theorem, as it grows like $e^{\pi y}$ on the imaginary axis.

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- $W_n(s)$ satisfies the conditions of the theorem (and is in fact analytic for $\Re(s) > -2$ when $n > 2$).
- There is a lovely **1941** proof by Selberg of the bounded case.

Analytic continuation

- So integer recurrences yield complex functional equations. Viz

$$(s+4)^2 W_3(s+4) - 2(5s^2+30s+46) W_3(s+2) + 9(s+2)^2 W_3(s) = 0.$$

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- This gives analytic continuations of the ramble integrals to the complex plane, with poles at certain negative integers (likewise for all n).

"*For it is easier to supply the proof when we have previously acquired, by the method [of mechanical theorems], some knowledge of the questions than it is to find it without any previous knowledge.* — Archimedes.

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- This gives analytic continuations of the ramble integrals to the complex plane, with poles at certain negative integers (likewise for all n).
- $W_3(s)$ has a simple pole at -2 with residue $\frac{2}{\sqrt{3}\pi}$, and other simple poles at $-2k$ with residues a rational multiple of Res_{-2}.

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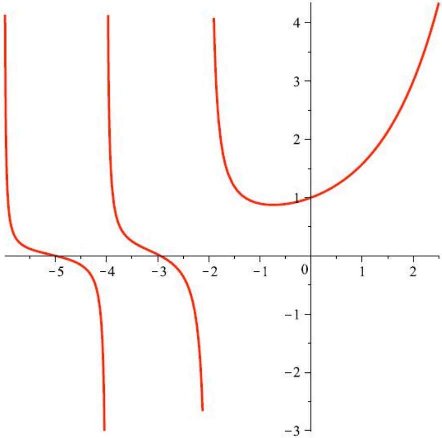
Odd dimensions look like 3

$W_3(s)$ on $[-6, \frac{5}{2}]$



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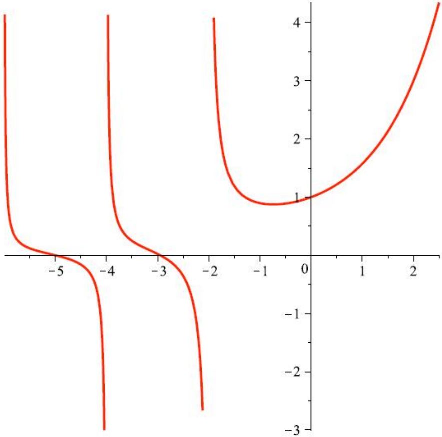

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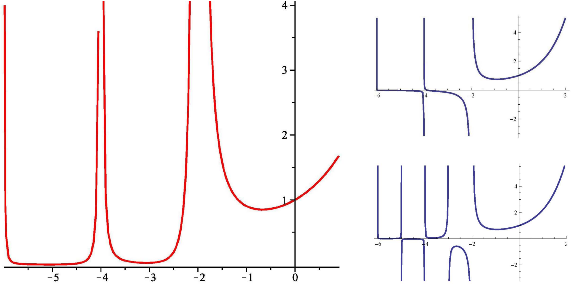
Some even dimensions look more like 4



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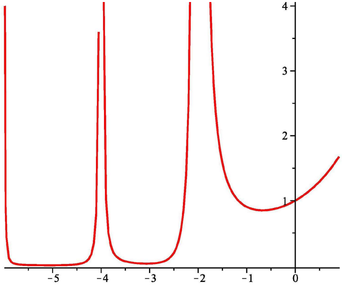

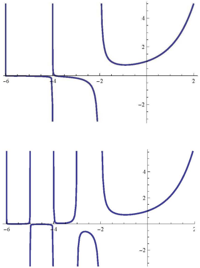

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$$\begin{aligned}(s+4)^3W_4(s+4) &- 4(s+3)(5s^2+30s+48)W_4(s+2)\\ &+ 64(s+2)^3W_4(s)=0\end{aligned}$$

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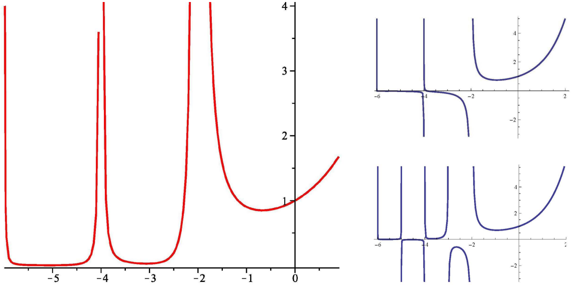

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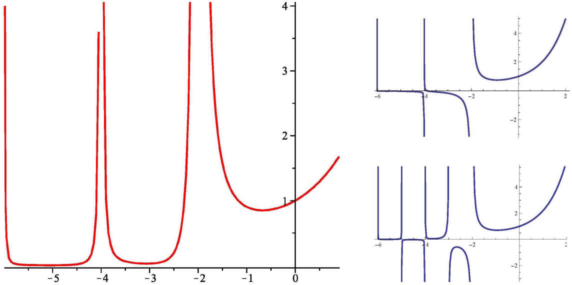

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- There are (infinitely many) multiple poles if and only if $4|n$.
- Why is W_4 positive on $\mathbf{R}$?

A discovery demystified

In particular, we have now shown that

$$W_3(2k) = \sum_{a_1+a_2+a_3=k} \binom{k}{a_1, a_2, a_3}^2 = \underbrace{{}_3F_2\left(\begin{matrix}1/2, -k, -k\\ 1, 1\end{matrix}\middle| 4\right)}_{=: V_3(2k)}$$

where ${}_pF_q$ is the generalized hypergeometric function. We discovered *numerically* that: $V_3(1) = 1.57459 - .12602652i$

Theorem (Real part)

For all integers k we have $W_3(k) = \Re(V_3(k))$.

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Theorem (Real part)

For all integers k we have $W_3(k) = \Re(V_3(k))$.

We have a habit in writing articles published in scientific journals to make the work as finished as possible, to cover up all the tracks, to not worry about the blind alleys or describe how you had the wrong idea first. . . . So there isn't any place to publish, in a dignified manner, what you actually did in order to get to do the work. — Richard Feynman (Nobel acceptance 1966)

Proof with hindsight

$k = 1$. From a dimension reduction, and elementary manipulations,

$$\begin{aligned} W_3(1) &= \int_0^1 \int_0^1 \left|1 + e^{2\pi i x} + e^{2\pi i y}\right| \mathrm{d}x \mathrm{d}y \\ &= \int_0^1 \int_0^1 \sqrt{4 \sin(2\pi t) \sin(2\pi(s + t/2)) - 2\cos(2\pi t) + 3}\, \mathrm{d}s \mathrm{d}t. \end{aligned}$$

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$$\begin{aligned} W_3(1) &= \int_0^1 \int_0^1 \left|1 + e^{2\pi i x} + e^{2\pi i y}\right| \mathrm{d}x\mathrm{d}y \\ &= \int_0^1 \int_0^1 \sqrt{4 \sin(2\pi t) \sin(2\pi(s + t/2)) - 2\cos(2\pi t) + 3}\, \mathrm{d}s\mathrm{d}t. \end{aligned}$$

- Let $s + t/2 \to s$, and use periodicity of the integrand, to obtain

$$W_3 = \int_0^1 \left\{ \int_0^1 \sqrt{4\cos(2\pi s)\sin(\pi t) - 2\cos(2\pi t) + 3}\, \mathrm{d}s \right\} \mathrm{d}t.$$

The inner integral can now be computed because

$$\int_0^\pi \sqrt{a + b\cos(s)}\, \mathrm{d}s = 2\sqrt{a+b}\; E\left(\sqrt{\frac{2b}{a+b}}\right).$$

Proof continued

Here $E(x)$ is the elliptic integral of the second kind:

$$E(x) := \int_0^{\pi/2} \sqrt{1 - x^2 \sin^2(t)}\, \mathrm{d}x.$$

- After simplification,

$$W_3 = \frac{4}{\pi^2} \int_0^{\pi/2} (2\sin(t) + 1) E\left(\frac{2\sqrt{2\sin(t)}}{1 + 2\sin(t)}\right) \mathrm{d}t.$$

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Now we recall Jacobi's imaginary transform,

$$(x+1)E\left(\frac{2\sqrt{x}}{x+1}\right) = \Re(2E(x) - (1 - x^2)K(x))$$

and substitute. Here $K(x)$ is the elliptic integral of the first kind.

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- This is where $\Re$ originates:
- e.g., $V_3(-1) = 0.896441 - 0.517560i, W_3(-1) = 0.896441.$

Proof completed

Using the integral definition of K and E, we can express W_3 as a double integral involving only $\sin$. Set

$$\Omega_3(a) := \frac{4}{\pi^2} \int_0^{\pi/2} \int_0^{\pi/2} \frac{1 + a^2 \sin^2(t) - 2\, a^2 \sin^2(t) \sin^2(r)}{\sqrt{1 - a^2 \sin^2(t) \sin^2(r)}} \, \mathrm{d}t \mathrm{d}r,$$

so that

$$\Re(\Omega_3(2)) = W_3(1). \tag{3}$$

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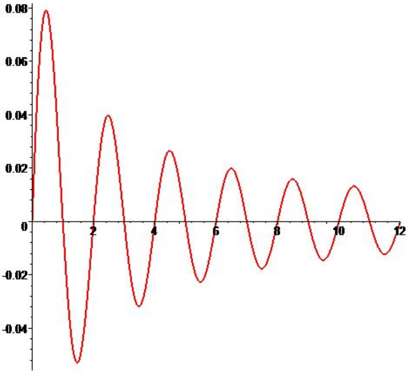
- As both sides satisfy the same 2-term recursion (computer provable), we are done. **QED**

A pictorial 'proof' shows Carlson's theorem does not apply

$W_3(s) - \Re V_3(s)$ on $[0, 12]$



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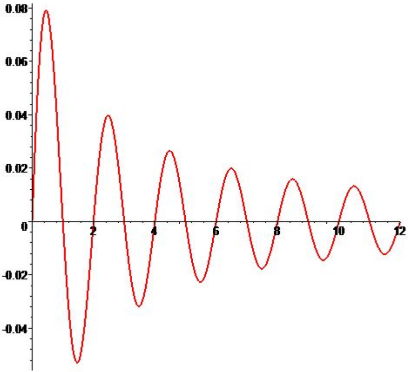

- This was hard to draw when discovered, as at the time we had no good closed form for W_3 (computational or hyper-closed).

Closed forms

- We then *confirmed* 175 digits of

$$W_3(1) \approx 1.57459723755189365749\ldots$$

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- Obtained via singular values of the elliptic integral and Legendre's identity.

Meijer-G functions (1936–)

Definition

$$G^{m,n}_{p,q}\left(\begin{matrix}a_1,\ldots,a_p\\ b_1,\ldots,b_q\end{matrix}\,\middle|\,x\right) := \frac{1}{2\pi i}\times$$

$$\int_L \frac{\prod_{j=1}^m \Gamma(b_j-s)\prod_{j=1}^n \Gamma(1-a_j+s)}{\prod_{j=n+1}^p \Gamma(a_j-s)\prod_{j=m+1}^q \Gamma(1-b_j+s)} x^s \mathrm{d}s.$$

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- Contour L chosen so it lies between poles of $\Gamma(1-a_i-s)$ and of $\Gamma(b_i+s)$.
- A broad generalization of hypergeometric functions — capturing Bessel Y, K and much more.
- Important in CAS, they often lead to superpositions of hypergeometric terms.

Meijer-G forms for W_3 and W_4

Theorem (Meijer form for W_3)

For s not an odd integer

$$W_3(s) = \frac{\Gamma(1+\frac{s}{2})}{\sqrt{\pi}\,\Gamma(-\frac{s}{2})}\, G^{21}_{33}\left(\begin{matrix}1,1,1\\ \frac{1}{2},-\frac{s}{2},-\frac{s}{2}\end{matrix}\,\middle|\,\frac{1}{4}\right).$$

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- $W_3(s)$ is among the first non-trivial higher order Meijer-G function to be placed in closed form.

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The most important aspect in solving a mathematical problem is the conviction of what is the true result. Then it took 2 or 3 years using the techniques that had been developed during the past 20 years or so. — Lennart Carleson (From 1966 IMU address on his positive solution of Luzin's problem).

Meijer-G form for W_4

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For $\Re s > -2$ and s not an odd integer

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- Not helpful for odd integers. We must again look elsewhere ...

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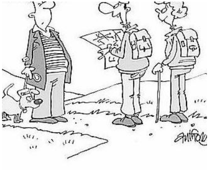

"WE'RE LOOKING FOR OUR *LOCAL* POST OFFICE"

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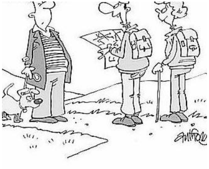
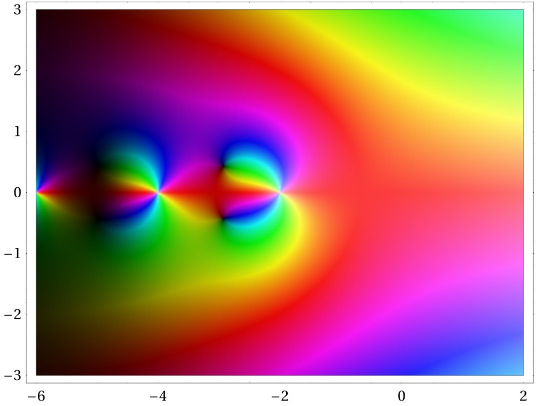


"WE'RE LOOKING FOR OUR *LOCAL* POST OFFICE"

He [Gauss (or Mma)] is like the fox, who effaces his tracks in the sand with his tail.— Niels Abel (1802-1829)

Visualizing W_4 in the complex plane



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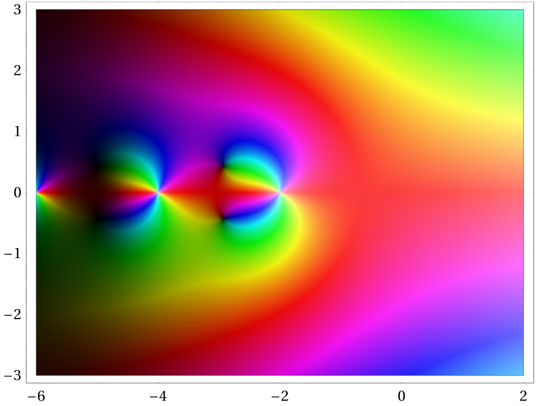

- Easily drawn now in *Mathematica* from the the Meijer-G representation.

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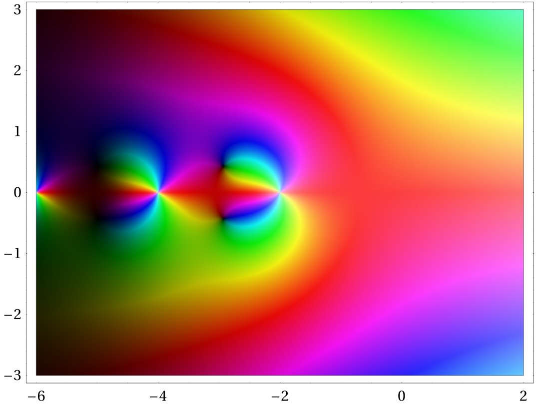


- Easily drawn now in *Mathematica* from the the Meijer-G representation.
- Each point is coloured differently (black is zero and white infinity). Note the poles and zeros.

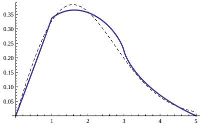
IV. PROBABILITY

It can be readily shown that

$$P_n(r) = \int_0^\infty r\, J_1(ry)\, [J_o(y)]^n \, dy \qquad (1.2)$$

where $J_k(y)$ is the Bessel function of the first kind of order k. Pearson tabulated $F_n(r)/2$ for $n \le 7$, for r ranging between 0 and n (all that is necessary). He used a graphical procedure in getting his results, and remarked that for $n = 5$ the function appeared to be constant over the range between 0 and 1. He states: 'From $r = 0$ to $r = L$ (here 1) the graphical construction, however carefully reinvestigated, did not permit of our considering the curve to be anything but a *straight* line. . . . Even if it is not absolutely true, it exemplifies the extraordinary power of such integrals of J products to give extremely close approximations to such simple forms as horizontal lines.'

Greenwood and Duncan (Reference [4]) later extended Pearson's work for n=6(1)24, and more recently Scheid (Reference [5]) gave results for lower values of n (2 to 6) obtained by a Monte Carlo procedure. The function $F_5(r)$ was computed for $r < 1$ on the Remington-Rand 1103 computer. The results are given in Table 1, and although the function is not constant, it differs from 1/3 by less than .0034 in this range. This settles Pearson's conjecture. The table given on page 51 may help investigators of Monte Carlo techniques to compare their results with the known values.



H.E. Fettis (1963)
"On a [1906] conjecture of Pearson."

Alternative representations

In **1906** the influential Leiden mathematician J.C. Kluyver (1860-1932) published a *fundamental* Bessel representation for the cumulative radial distribution function (P_n) and density (p_n) of the distance after n-steps:

$$P_n(t) = t \int_0^\infty J_1(xt)\, J_0^n(x)\, \mathrm{d}x$$

$$p_n(t) = t \int_0^\infty J_0(xt)\, J_0^n(x) x\, \mathrm{d}x \quad (n \geq 4) \tag{6}$$

where $J_n(x)$ is the Bessel J function of the first kind (see Watson (1932, §49); 3-dim walks are *elementary*).

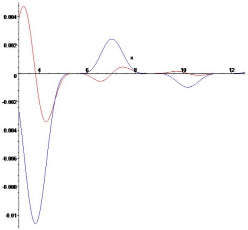
- From (8) below, we find

$$p_n(1) = \mathrm{Res}_{-2}\left(W_{n+1}\right) \qquad (n \neq 4). \tag{7}$$

- As $p_2(\alpha) = \frac{2}{\pi\sqrt{4-\alpha^2}}$, we check in *Maple* that the following code returns $R = 2/(\sqrt{3}\pi)$ *symbolically*:

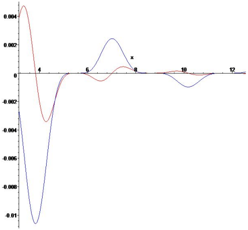
```
R:=identify(evalf[20](int(BesselJ(0,x)^3*x,x=0..infinity)))
```

A Bessel integral for W_n



A Bessel integral for W_n

- Also $P_n(1) = \frac{J_0(0)^{n+1}}{n+1} = \frac{1}{n+1}$ (Pearson's original question).



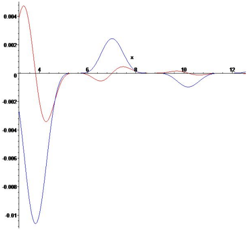
A Bessel integral for W_n

- Also $P_n(1) = \frac{J_0(0)^{n+1}}{n+1} = \frac{1}{n+1}$ (Pearson's original question).
- Broadhurst used (6) to show for $2k > s > -\frac{n}{2}$ that

$$W_n(s) = 2^{s+1-k} \frac{\Gamma(1+\frac{s}{2})}{\Gamma(k-\frac{s}{2})} \int_0^\infty x^{2k-s-1} \left(-\frac{1}{x}\frac{\mathrm{d}}{\mathrm{d}x}\right)^k J_0^n(x)\mathrm{d}x, \tag{8}$$

a useful oscillatory 1-dim integral (used below). Thence

$$W_n(-1) = \int_0^\infty J_0^n(x)\mathrm{d}x, \;\; W_n(1) = n\int_0^\infty J_1(x)J_0(x)^{n-1}\frac{\mathrm{d}x}{x}. \tag{9}$$



Integrands for $W_4(-1)$ (blue) and $W_4(1)$ (red) on $[\pi, 4\pi]$ from (9).

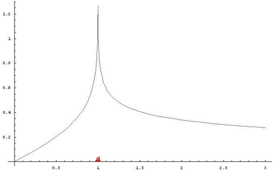
The densities for $n = 3, 4$ are modular (JW's talk)

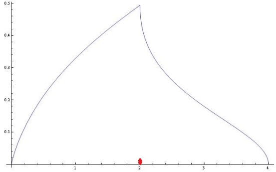
Let $\sigma(x) := \frac{3-x}{1+x}$. Then σ is an involution on $[0, 3]$ sending $[0, 1]$ to $[1, 3]$:

$$p_3(x) = \frac{4x}{(3-x)(x+1)}\, p_3(\sigma(x)). \tag{10}$$

So $\frac{3}{4}p_3'(0) = p_3(3) = \frac{\sqrt{3}}{2\pi}, p(1) = \infty$. We found:

The densities p_3 (L) and p_4 (R)





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$$p_3(\alpha) = \frac{2\sqrt{3}\alpha}{\pi\,(3+\alpha^2)}\, {}_2F_1\left(\begin{matrix}\frac{1}{3}, \frac{2}{3}\\ 1\end{matrix}\,\middle|\, \frac{\alpha^2\left(9-\alpha^2\right)^2}{\left(3+\alpha^2\right)^3}\right) = \frac{2\sqrt{3}}{\pi}\,\frac{\alpha}{\mathrm{AG}_3(3+\alpha^2, 3\left(1-\alpha^2\right)^{2/3})} \tag{11}$$

where AG_3 is the *cubically convergent* mean iteration (1991):

$$\mathrm{AG}_3(a, b) := \frac{a+2b}{3} \bigotimes \left(b \cdot \frac{a^2+ab+b^2}{3}\right)^{1/3}$$

.

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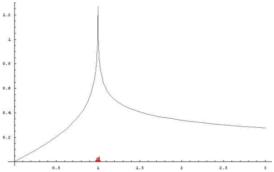
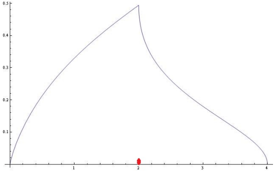
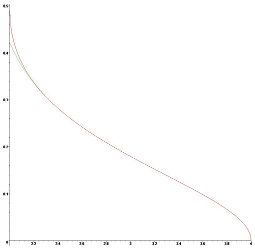




Formula for the ‘shark-fin’ p_4 (stimulated by S. Robins)

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

$$p_4(\alpha) = \frac{2}{\pi^2} \frac{\sqrt{16-\alpha^2}}{\alpha} \, {}_3F_2\left({\frac{1}{2}, \frac{1}{2}, \frac{1}{2} \atop \frac{5}{6}, \frac{7}{6}} \middle| \frac{\left(16-\alpha^2\right)^3}{108\,\alpha^4} \right). \tag{12}$$



- ← p_4 from (12) vs 18-terms of empirical power series
- ✓ Proves $p_4(2) = \frac{2^{7/3}\pi}{3\sqrt{3}} \Gamma\left(\frac{2}{3}\right)^{-6} = \frac{\sqrt{3}}{\pi} W_3(-1) \approx 0.494233 < \frac{1}{2}$
- Empirically, quite marvelously, we found — and proved by a subtle use of distributional Mellin transforms — that on $[0, 2]$ as well:

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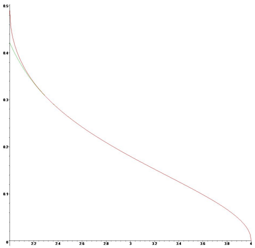

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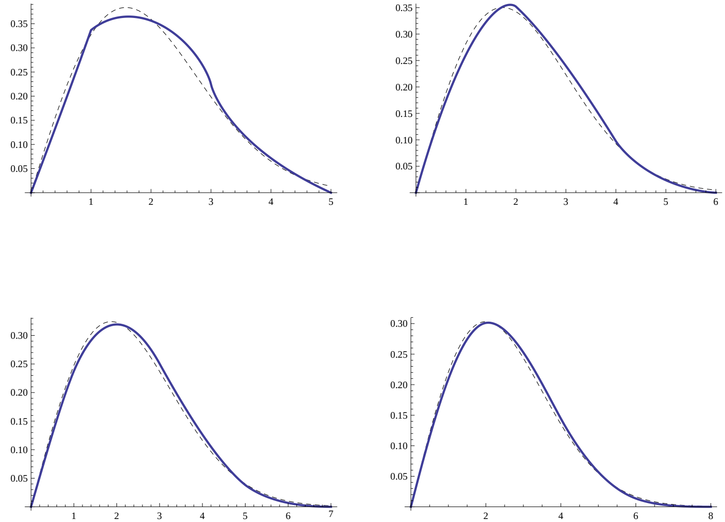
(Discovering this $\Re$ brought us full circle.)

The densities for $5 \leq n \leq 8$ (and large n approximation)



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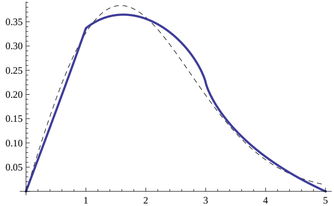
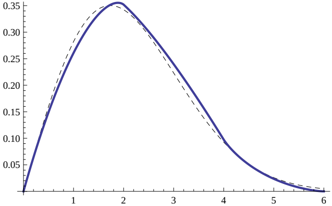
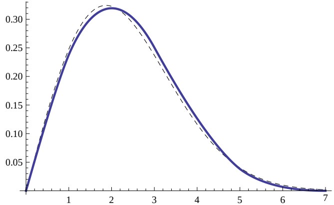
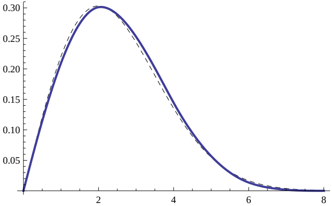




- Both p_{2n+4}, p_{2n+5} are n-times continuously differentiable for $x > 0$ $\left(p_n(x) \sim \frac{2x}{n} e^{-x^2/n}\right)$. So "four is small" *but* "eight is large."





Simplifying the Meijer integral

- We (humans and computers) now obtained:

Corollary (Hypergeometric forms for noninteger $s > -2$)

$$W_3(s) = \frac{1}{2^{2s+1}} \tan\left(\frac{\pi s}{2}\right) \binom{s}{\frac{s-1}{2}}^2 {}_3F_2\left(\left. {\frac{1}{2}, \frac{1}{2}, \frac{1}{2} \atop \frac{s+3}{2}, \frac{s+3}{2}} \right| \frac{1}{4} \right) + \binom{s}{\frac{s}{2}} {}_3F_2\left(\left. {-\frac{s}{2}, -\frac{s}{2}, -\frac{s}{2} \atop 1, -\frac{s-1}{2}} \right| \frac{1}{4} \right),$$

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- We (humans) were able to provably take the limit:

$$W_4(-1) = \frac{\pi}{4}\, {}_7F_6\left({\frac{5}{4}, \frac{1}{2}, \frac{1}{2}, \frac{1}{2}, \frac{1}{2}, \frac{1}{2}, \frac{1}{2} \atop \frac{1}{4}, 1, 1, 1, 1, 1} \middle| 1 \right) = \frac{\pi}{4} \sum_{n=0}^{\infty} \frac{(4n+1)\binom{2n}{n}^6}{4^{6n}}$$

$$= \frac{\pi}{4}\, {}_6F_5\left({\frac{1}{2}, \frac{1}{2}, \frac{1}{2}, \frac{1}{2}, \frac{1}{2}, \frac{1}{2} \atop 1, 1, 1, 1, 1} \middle| 1 \right) + \frac{\pi}{64}\, {}_6F_5\left({\frac{3}{2}, \frac{3}{2}, \frac{3}{2}, \frac{3}{2}, \frac{3}{2}, \frac{3}{2} \atop 2, 2, 2, 2, 2} \middle| 1 \right).$$

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- We have proven the corresponding result for $W_4(1)$ ....

An elliptic integral harvest

Indeed, PSLQ found various representations including:

$$W_4(1) = \frac{9\pi}{4}\,{}_7F_6\left(\left.\begin{matrix}\frac{7}{4},\frac{3}{2},\frac{3}{2},\frac{3}{2},\frac{1}{2},\frac{1}{2},\frac{1}{2}\\ \frac{3}{4},2,2,2,1,1\end{matrix}\right|1\right) - 2\pi\,{}_7F_6\left(\left.\begin{matrix}\frac{5}{4},\frac{1}{2},\frac{1}{2},\frac{1}{2},\frac{1}{2},\frac{1}{2},\frac{1}{2}\\ \frac{1}{4},1,1,1,1,1\end{matrix}\right|1\right)$$

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- Proofs rely on work by Nesterenko and by Zudilin. Inter alia:

$$2\int_0^1 K(k)^2\mathrm{d}k = \int_0^1 K'(k)^2\mathrm{d}k = \left(\frac{\pi}{2}\right)^4\,{}_7F_6\left(\left.{\frac{5}{4},\frac{1}{2},\frac{1}{2},\frac{1}{2},\frac{1}{2},\frac{1}{2},\frac{1}{2} \atop \frac{1}{4},1,1,1,1,1}\right|1\right).$$

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- We also deduce that (K', E' are complementary integrals)

$$W_4(-1) = \frac{8}{\pi^3}\int_0^1 K^2(k)\mathrm{d}k\; W_4(1) = \frac{96}{\pi^3}\int_0^1 E'(k)K'(k)\mathrm{d}k - 8\,W_4(-1).$$

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- Much else about moments of products of elliptic integrals has been discovered (with massive **1600** relation PSLQ runs)

Final refinements

Theorem (Moments of W_3)

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

$$W_3(s) = \frac{3^{s+3/2}}{2\pi} \beta\left(s+\frac{1}{2}, s+\frac{1}{2}\right) {}_3F_2\left({\frac{s+2}{2}, \frac{s+2}{2}, \frac{s+2}{2} \atop 1, \frac{s+3}{2}} \middle| \frac{1}{4} \right). \tag{14}$$

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

$$W_3(-2k-1) = \frac{\sqrt{3}\binom{2k}{k}^2}{2^{4k+1}3^{2k}} {}_3F_2\left({\frac{1}{2}, \frac{1}{2}, \frac{1}{2} \atop k+1, k+1} \middle| \frac{1}{4} \right),$$

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Likewise, we may improve (5) and show for *all* s,

$$W_4(s) = \frac{2^{2s+1}}{\pi^2\,\Gamma(\frac{s+2}{2})^2}\, G^{2,4}_{4,4}\left(\left.\begin{matrix} 1, 1, 1, \frac{s+3}{2} \\ \frac{s+2}{2}, \frac{s+2}{2}, \frac{s+2}{2}, \frac{1}{2} \end{matrix}\right| 1\right). \tag{15}$$

Derivative values also follow

From the hypergeometric forms of the corollary we get:

$$W_3'(0) = \frac{1}{\pi} {}_3F_2\left({\frac{1}{2}, \frac{1}{2}, \frac{1}{2} \atop \frac{3}{2}, \frac{3}{2}} \middle| \frac{1}{4} \right) = \frac{1}{\pi} \operatorname{Cl}\left(\frac{\pi}{3}\right). \tag{16}$$

The last equality follows from setting $\theta = \pi/6$ in the identity

$$2\sin(\theta)\,{}_3F_2\left({\frac{1}{2}, \frac{1}{2}, \frac{1}{2} \atop \frac{3}{2}, \frac{3}{2}} \middle| \sin^2\theta \right) = \operatorname{Cl}(2\theta) + 2\theta \log(2\sin\theta)$$

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Here $\operatorname{Cl}(\theta) := \sum_{n=1}^{\infty} \frac{\sin(n\theta)}{n^2}$ is *Clausen's function*. Likewise:

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...

V. OPEN PROBLEMS








Who are we? **Answers** (clockwise) **FD, AB, JvN, EW, HW, YM**

Open problems (Mahler measures, I)

Tantalizing parallels link the ODE methods we used for p_4 to those for the logarithmic *Mahler measure* of a polynomial P in n-space:

$$\mu(P) := \int_0^1 \int_0^1 \cdots \int_0^1 \log \left| P\left(e^{2\pi i\theta_1}, \cdots, e^{2\pi i\theta_n}\right) \right| d\theta_1 \cdots d\theta_n.$$

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Indeed

$$\mu\left(1 + \sum_{k=1}^{n-1} x_k\right) = W_n'(\mathbf{0}). \tag{18}$$

which we have evaluated in (16), (17) for $n = 3$ and $n = 4$ respectively.

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$$\mu(P) := \int_0^1 \int_0^1 \cdots \int_0^1 \log\left|P\left(e^{2\pi i\theta_1}, \cdots, e^{2\pi i\theta_n}\right)\right| d\theta_1 \cdots d\theta_n.$$

Indeed

$$\mu\left(1 + \sum_{k=1}^{n-1} x_k\right) = W_n'(\mathbf{0}). \tag{18}$$

which we have evaluated in (16), (17) for $n = 3$ and $n = 4$ respectively.

- $\mu(P)$ turns out to be an example of a **period**. When $n = 1$ and P has integer coefficients $\exp(\mu(P))$ is an algebraic integer. In several dimensions life is harder.

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- There are remarkable recent results — many more discovered than proven — expressing $\mu(P)$ arithmetically.

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- $\mu(1+x+y) = L_3'(-1) = \frac{1}{\pi}\,\mathrm{Cl}\left(\frac{\pi}{3}\right)$ (Smyth).
- $\mu(1+x+y+z) = 14\,\zeta'(-2) = \frac{7}{2}\,\frac{\zeta(3)}{\pi^2}$ (Smyth).

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  - Similarly for (18) $(n=5,6)$ conjectures of Villegas become:

$$W_5'(0) \stackrel{?}{=} \left(\frac{15}{4\pi^2}\right)^{5/2} \int_0^\infty \left\{\eta^3(e^{-3t})\eta^3(e^{-5t}) + \eta^3(e^{-t})\eta^3(e^{-15t})\right\} t^3\,\mathrm{d}t$$

$$W_6'(0) \stackrel{?}{=} \left(\frac{3}{\pi^2}\right)^{3} \int_0^\infty \eta^2(e^{-t})\eta^2(e^{-2t})\eta^2(e^{-3t})\eta^2(e^{-6t})\,t^4\,\mathrm{d}t$$

and Dedekind's η is $\eta(q) := q^{1/24}\sum_{n=-\infty}^{\infty}(-1)^n q^{n(3n+1)/4}$.

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We have proven:

$$W_4(2k) = \sum_{a_1+\cdots+a_4=k} \binom{k}{a_1,\ldots,a_4}^2$$

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Conjecture

For all integers k we have $W_4(k) = \Re(V_4(k))$.

Open problems (general n)

- Conjecture (19) is explained = "almost" proved — via residue calculus from Meijer-G form — modulo a technical growth estimate (**G**). For complex s and $n = 1, 2, \ldots$,

$$W_{2n}(s) \stackrel{?}{=} \sum_{j \geq 0} \binom{s/2}{j}^2 W_{2n-1}(s-2j). \tag{19}$$

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✓ *Could* confirm $n = 4, 5, 6, \ldots$ symbolically as we shall for $n = 3$:

Open problems ($n = 5$)

- The functional equation for W_5 is:

$$\begin{aligned} & 225(s+4)^2(s+2)^2 W_5(s) = -(35(s+5)^4 + 42(s+5)^2 + 3) W_5(s+4) \\ + \quad & (s+6)^4 W_5(s+6) + (s+4)^2(259(s+4)^2 + 104) W_5(s+2). \end{aligned}$$

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- From here we deduce *the first two poles* — and so all — *are simple* since

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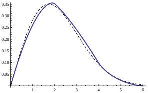

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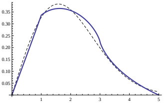
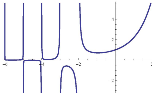


Laurent expansion *explains* puzzling (near) linearity of p_5 on $[0, 1]$.

$$p_5(1) = \mathrm{Res}_{(-2)}(W_6)$$

W_6 on $[-6, 2]$



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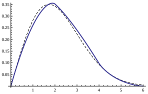

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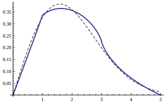

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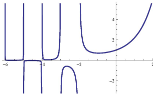

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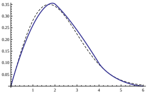

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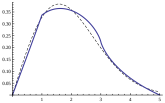

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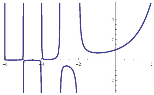

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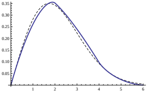

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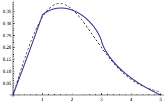

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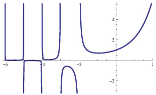

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- Here $r_5(k) := \mathrm{Res}_{(-2k)}(W_5)$. Other residues are then combinations as follows:
- From the W_5-recursion: given $r_5(0) = 0, r_5(1)$ and $r_5(2)$ we have

$$r_5(k+3) = \frac{k^4 r_5(k) - \left(5 + 28\,k + 63\,k^2 + 70\,k^3 + 35\,k^4\right) r_5(k+1)}{225(k+1)^2(k+2)^2} + \frac{\left(285 + 518\,k + 259\,k^2\right) r_5(k+2)}{225(k+2)^2}.$$

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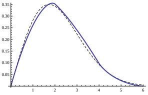

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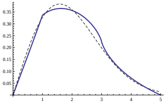

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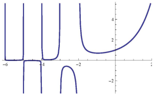


Open problems (computing derivatives of W_n)

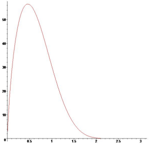
Maple2latex code for the symbolic derivatives $W_n^{(k)}(s)$ is as follows:

```
WN:=proc (N,s,k) local t,j,dk; dk:=BesselJ(0,t)^N;
    for j from 1 to k do dk:=-1/t*diff(dk,t) od;
    2^(s-k+1)*GAMMA(s/2+1)/GAMMA(k-s/2)
    *Int(t^(2*k-s-1)*dk,t = 0 .. infinity);end;
>latex(normal(combine(simplify(subs(s=4,diff(WN(5,s,3),s))
```

Prettified this yields $W_5'(4) = 40 \int_0^\infty f(t)\,\mathrm{d}t$ where $f(t) :=$

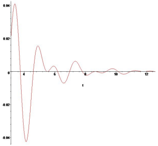
$$\frac{\left\{8\,\mathrm{J}_0^4(t)\mathrm{J}_1(t) + 24\,\mathrm{J}_0^3(t)\mathrm{J}_1^2(t)t - 4\,\mathrm{J}_0^5(t)t + 12\,\mathrm{J}_0^2(t)\mathrm{J}_1^3(t)t^2 - 13\,\mathrm{J}_0^4(t)\mathrm{J}_1(t)t^2\right\}\left(\log\left(\frac{2}{t}\right) - \gamma + \frac{3}{4}\right)}{t^4}$$

f on $[0, \pi]$



Effective computation of Bessel integrals (e.g., Lucas–Stone 95) to high or extreme precision is an ongoing project with Bailey. (Needed for any substantial use of PSLQ.)

f on $[\pi, 4\pi]$



Thank you ...

Two ramblers at ANZIAM 2010

Thank you ...

Conclusion. We continue to be fascinated by this blend of combinatorics, number theory, analysis, probability, and differential equations, all tied together with experimental mathematics.

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