Moments and Densities of Short Random Walks

in all Dimensions

Jonathan M. Borwein FRSC FAAAS FBAS FAA FAMS
Joint with Armin Straub, James Wan, (Christophe Vignat), Wadim Zudilin, ...

Director, CARMA, the University of Newcastle

September 18–19, 2015

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From Mathematical Beauties, Calendar (August 2016)

Number Theory Down Under

18-19 September, 2015
The University of Newcastle

It is our great pleasure to announce that the Centre for Computer-Assisted Research Mathematics and its Applications (CARMA) will be hosting a two-day number theory workshop **Number Theory Down Under (NTDU)** on 18th and 19th September 2015, at the University of Newcastle. The talks will be in the lecture theatre VG01. Links for the previous meetings are available here NTDU13 and NTDU14 and a bunch of **photographs.**

Details about registration, confirmed participants, accommodation, travel, and anything else needed can be found below.

If you have any questions, please email Mumtaz Hussain at Mumtaz.Hussain@newcastle.edu.au

AMSI AUSTRALIAN MATHEMATICAL SCIENCES INSTITUTE

CARMA

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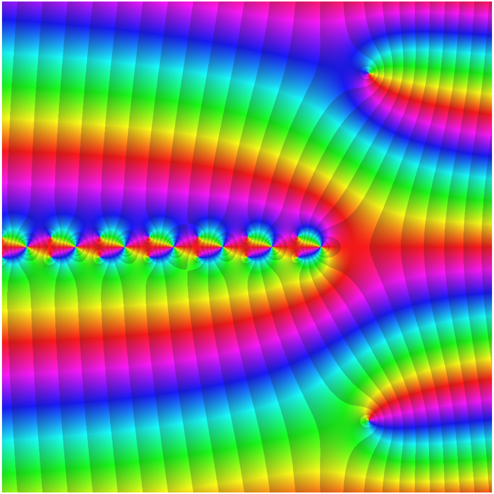

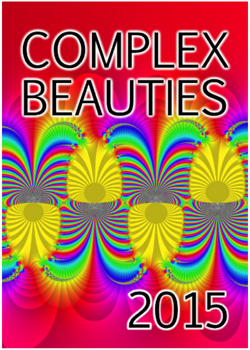

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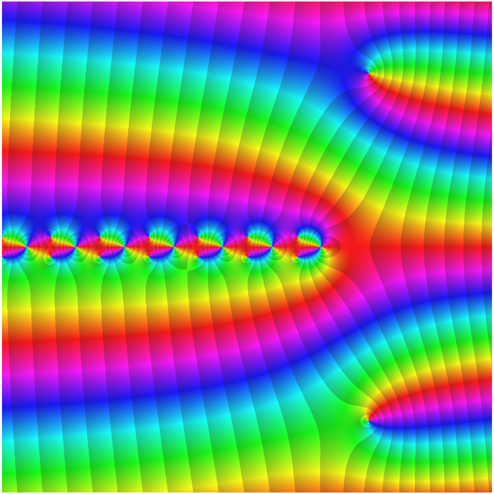

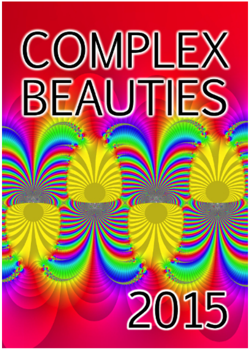

- The (complex) moment function of a 4-step walk in the plane.

Outline

I. INTRODUCTION

- An age old question: What is a walk?

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- Also (self-avoiding) random walks, random migrations, random flights.

Abstract

Following Pearson in **1905**, we first study the expected distance and density of a two-dimensional walk in the plane with n unit steps in random directions — what Pearson called a random walk. We finish by examining our prior work in higher dimensions.

- We present recent results on the densities, p_n, of n-step random uniform random walks in the plane ($d := 2\nu + 2 = 2$).
- For $n \geq 7$ asymptotic formulas first developed by Raleigh are *largely* sufficient to describe the density.

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- We shall see remarkable new hypergeometric closed forms for p_3, p_4 and precise analytic information for larger n.
- Heavy use is made of analytic continuation of the integral (also of modern special functions (e.g., Meijer-G) and computer algebra (CAS)).

I. Random walk integrals — our starting point

For complex s

Definition (Moment function)

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

- W_n is analytic precisely for $\Re s > -2$.
- Also, $W_n(1)$ is 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:

$$W_2(1) = \int_0^1 \int_0^1 \left| e^{2\pi i x} + e^{2\pi i y} \right| \mathrm{d}x \mathrm{d}y = \ ?$$

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

$n \geq 3$ 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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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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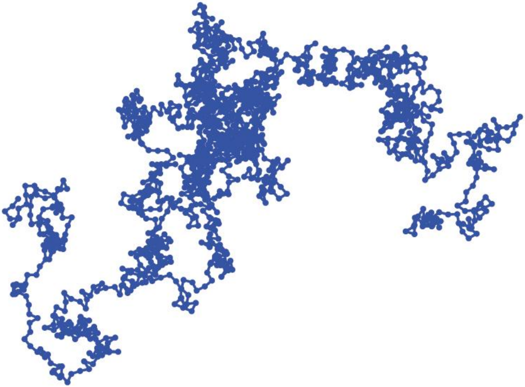
One 1500-step ramble: ...a familiar picture



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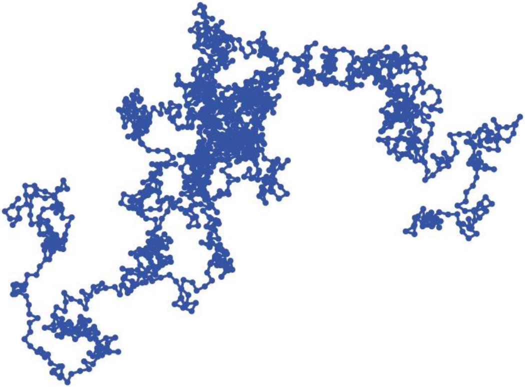

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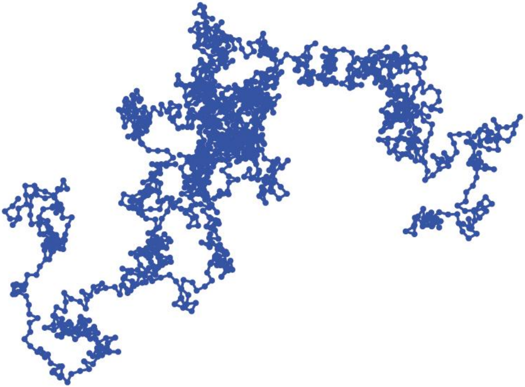
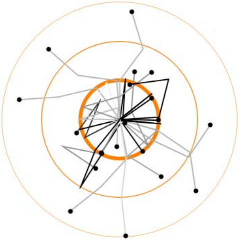


- 1D (and 3D) easy. Expectation of RMS distance is easy ($\sqrt{n}$).
- 1D or 2D *lattice*: probability one of returning to the origin.
  Drunken men get home, birds do not (Kakutani)

1000 three-step rambles: ... a less familiar picture?



The long and the short of it

A little history — — from a vast literature

L: Pearson posed question (*Nature*, 1905).

R: Rayleigh gave large n asymptotics: $p_n(x) \sim \frac{2x}{n} e^{-x^2/n}$ (*Nature*, 1905).

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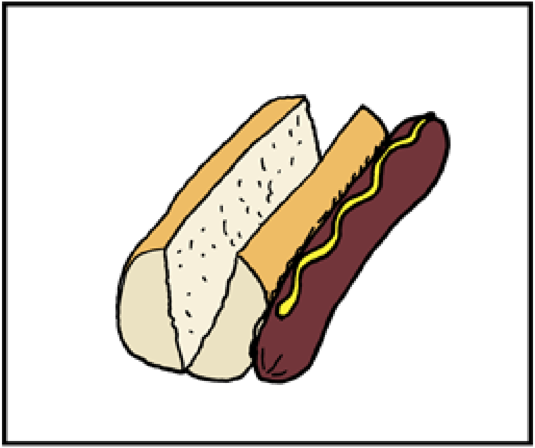
- Appear in quantum chemistry, in quantum physics as hexagonal and diamond lattice integers, etc ...

II. COMBINATORICS



REVERSE POLISH SAUSAGE

$W_n(k)$ 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
$W_4(k)$	1	4	28	256	2716	31504
$W_5(k)$	1	5	45	545	**7885**	**127905**

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- *MathWorld* gives $W_n(2) = n$ (trivial).
- Entering `1,5,45,545` in the *OEIS* now gives *"The function $W_5(2n)$ (see Borwein et al. reference for definition)."*

$W_n(k)$ at odd integers

n	$k=1$	$k=3$	$k=5$	$k=7$	$k=9$
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

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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):

$$W_n(2k) = \sum_{a_1+\ldots+a_n=k} \binom{k}{a_1,\ldots,a_n}^2. \qquad (1)$$

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

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

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- and recursions such as:

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

- $W_n(2k)$ satisfies an $\lfloor \frac{n+1}{2} \rfloor$-term recursion and $\lfloor \frac{n+3}{2} \rfloor$ distinct iterated sums.
- Also

$$\begin{aligned} W_3(1) &= 3\sum_{n=0}^{\infty}\binom{1/2}{n}\left(-\frac{8}{9}\right)^n\sum_{k=0}^{n}\binom{n}{k}\left(-\frac{1}{8}\right)^k\sum_{j=0}^{k}\binom{k}{j}^3 \\ &= 3\sum_{n=0}^{\infty}(-1)^n\binom{1/2}{n}\sum_{k=0}^{n}\binom{n}{k}\left(-\frac{1}{9}\right)^k\sum_{j=0}^{k}\binom{k}{j}^2\binom{2j}{j} \end{aligned}$$

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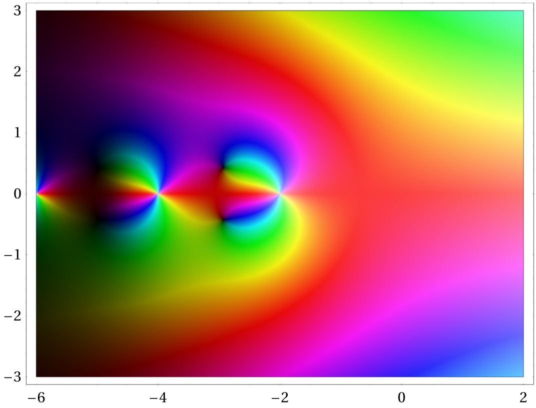
- Tanh-sinh (doubly-exponential) quadrature works well for W_3 but not so well for $W_4 \approx 1.79909248$.
- Quasi-Monte Carlo was *not* very accurate.

III. ANALYSIS

Visualizing W_4 in the complex plane



Carlson's theorem: ...from discrete to continuous

Theorem (Carlson (1914, PhD))

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

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

then $f(z) = 0$ identically in the region.

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

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- $|W_n(\nu; s)| \leq n^{|\Re(s)|}$ satisfies the conditions of the theorem (and $W_n(0; s)$ is in fact analytic for $\Re(s) > -2$ when $n > 2$).

Carlson's theorem: ...from discrete to continuous

Theorem (Carlson (1914, PhD))

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

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

then $f(z) = 0$ identically in the region.

- $\sin(\pi z)$ does not satisfy the conditions of the theorem, as it grows like $e^{\pi y}$ on the imaginary axis.
- $|W_n(\nu; s)| \leq n^{|\Re(s)|}$ satisfies the conditions of the theorem (and $W_n(0; s)$ 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).
- $W_3(s)$ 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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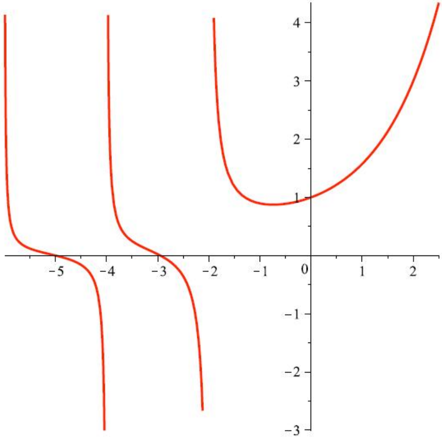
Odd lengths look like 3

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



- JW proved zeroes near *to* but *not at* integers: $W_3(-2n-1) \downarrow 0$.

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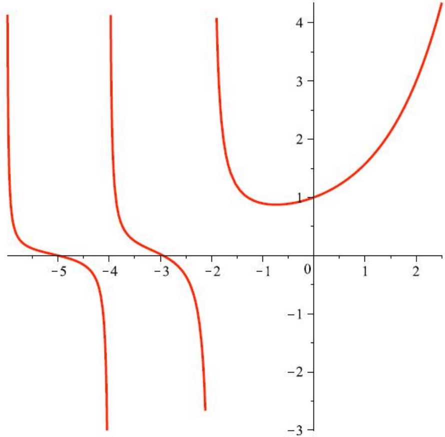

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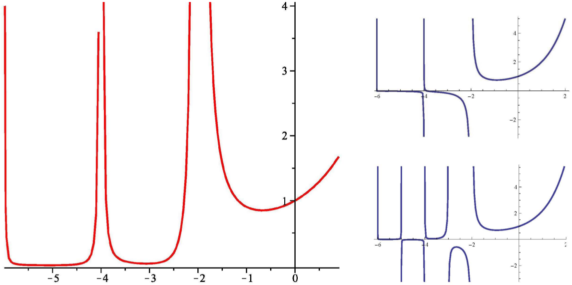

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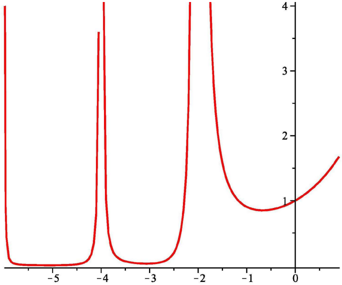

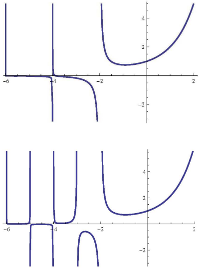

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- The functional equation (with double poles) for $n = 4$ is

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

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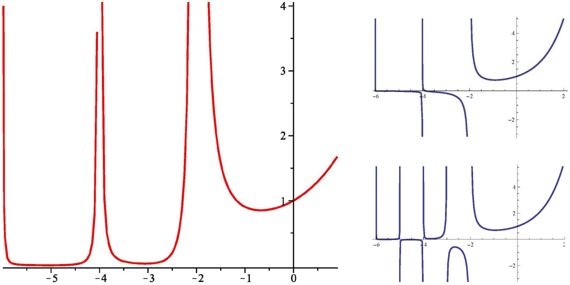

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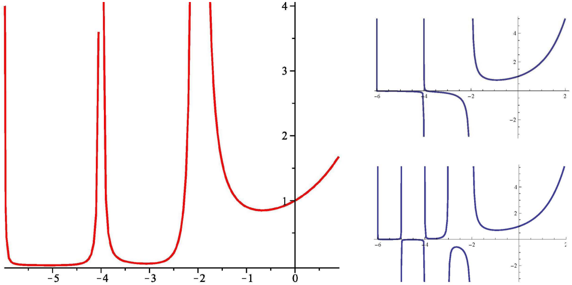

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- Conjecture: multiple poles iff $4|n$ (proven for small n).
- Why is W_4 positive on $\mathbf{R}$?

A discovery demystified

In particular, we had 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 (similarly in all even dimensions))

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

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

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

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,

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

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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

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

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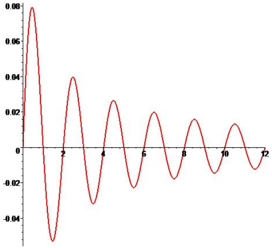
- As both sides satisfy the same 2-term recursion (computer provable), we are done. **QED**

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

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



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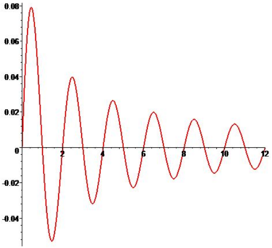

- This was hard to draw when discovered, as at the time we had no good closed form for $W_3(s)$. For $s \neq -3, -5, -7, \ldots$, we now have

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

Closed forms

- We then *confirmed* 175 digits of

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- Armed with a knowledge of elliptic integrals:

$$W_3(1) = \frac{16\sqrt[3]{4}\,\pi^2}{\Gamma(\frac{1}{3})^6} + \frac{3\Gamma(\frac{1}{3})^6}{8\sqrt[3]{4}\,\pi^4} = W3(-1) + \frac{6/\pi^2}{W3(-1)},$$

$$W_3(-1) = \frac{3\Gamma(\frac{1}{3})^6}{8\sqrt[3]{4}\,\pi^4} = \frac{2^{\frac{1}{3}}}{4\pi^2}\beta^2\left(\frac{1}{3}\right).$$

Here $\beta(s) := B(s,s) = \frac{\Gamma(s)^2}{\Gamma(2s)}$.

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

IV. PROBABILITY

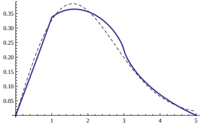
It can be readily shown that

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

where $J_k(y)$ is the Bessel function of the first kind of order k. Pearson tabulated $F_n(r)/2$ for $n \leq 7$, 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.

Since the function $F_5(r)$ is so nearly constant in the range between 0 and 1,



H.E. Fettis (1963)

"On a [1906] conjecture of Pearson."

The Bessel J function

Recall, the normalized Bessel function of the first kind is

$$j_\nu(x) = \nu! \left(\frac{2}{x}\right)^\nu J_\nu(x) = \nu! \sum_{m\geq 0} \frac{(-x^2/4)^m}{m!(m+\nu)!}. \tag{4}$$

With this normalization, we have $j_\nu(0) = 1$ and

$$j_\nu(x) \sim \frac{\nu!}{\sqrt{\pi}} \left(\frac{2}{x}\right)^{\nu+1/2} \cos\left(x - \frac{\pi}{2}\left(\nu + \frac{1}{2}\right)\right)$$

as $x \to \infty$ on the real line.

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as $x \to \infty$ on the real line.

- Note also that

$$j_{1/2}(x) = \mathrm{sinc}(x) = \sin(x)/x$$

– which in part explains why analysis in 3-space is so simple. More generally, all half-integer order $j_\nu(x)$ are elementary.

Richer representations

1906. The influential Leiden mathematician J.C. Kluyver (1860-1932) — supervisor of Kloosterman —published a *fundamental* Bessel representation for the cumulative radial distribution function (P_n) and density (p_n) :

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

$$p_n(t) = t \int_0^\infty J_0(xt)\, J_0^n(x) x\, \mathrm{d}x \quad (n \geq 4) \tag{5}$$

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

- From (7) below, we find

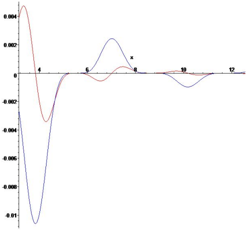
$$p_n(1) = \mathrm{Res}_{-2}\,(W_{n+1}) \qquad\qquad (n = 1, 2, \ldots). \tag{6}$$

- 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

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



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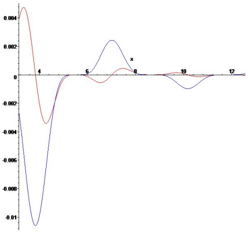


Integrands for $W_4(-1)$ (blue) and $W_4(1)$ (red) on $[\pi, 4\pi]$ from (8).

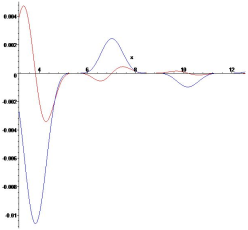
A Bessel integral for W_n

- Also $P_n(1) = \frac{J_0(0)^{n+1}}{n+1} = \frac{1}{n+1}$ (A question of Pearson).
- Broadhurst used (5) to show for $2k > s > -\frac{n}{2}$ that

$$W_n(s) = 2^{s+1-k} \frac{\Gamma(1+\frac{s}{2})}{\Gamma(k-\frac{s}{2})} \int_0^\infty x^{2k-s-1} \left(-\frac{1}{x}\frac{\mathrm{d}}{\mathrm{d}x}\right)^k J_0^n(x)\,\mathrm{d}x, \tag{7}$$

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

$$W_n(-1) = \int_0^\infty J_0^n(x)\,\mathrm{d}x, \;\; W_n(1) = n \int_0^\infty J_1(x) J_0(x)^{n-1} \frac{\mathrm{d}x}{x}. \tag{8}$$



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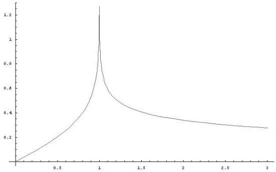
The densities for $n = 3, 4$ are 'modular'

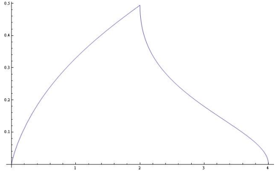
Let $\sigma(x) := \frac{3-x}{1+x}$. Then σ is an involution on $[0,3]$ sending $[0,1]$ to $[1,3]$:

$$p_3(x) = \frac{4x}{(3-x)(x+1)}\, p_3(\sigma(x)). \tag{9}$$

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

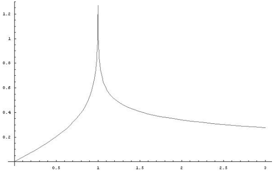
$$p_3(\alpha) = \frac{2\sqrt{3}\alpha}{\pi\,(3+\alpha^2)}\, {}_2F_1\left(\begin{matrix}\frac{1}{3}, \frac{2}{3}\\ 1\end{matrix}\,\middle|\, \frac{\alpha^2\left(9-\alpha^2\right)^2}{\left(3+\alpha^2\right)^3}\right) = \frac{2\sqrt{3}}{\pi}\, \frac{\alpha}{\mathrm{AG}_3\left(3+\alpha^2, 3\left(1-\alpha^2\right)^{2/3}\right)} \tag{10}$$

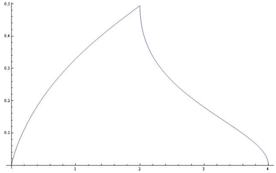
where AG_3 is the *cubically convergent* mean iteration (1991):

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

.

The densities p_3 (L) and p_4 (R)





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

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

$$p_4(\alpha) = \frac{2}{\pi^2} \frac{\sqrt{16-\alpha^2}}{\alpha} \, {}_3F_2\left(\left. \begin{matrix} \frac{1}{2}, \frac{1}{2}, \frac{1}{2} \\ \frac{5}{6}, \frac{7}{6} \end{matrix} \right| \frac{\left(16-\alpha^2\right)^3}{108\,\alpha^4} \right). \tag{11}$$

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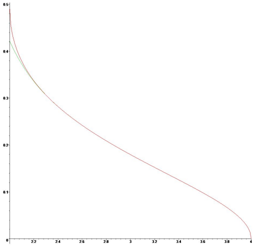

- ← p_4 from (11) vs 18-terms of empirical power series
- ✓ Proves $p_4(2) = \frac{2^{7/3}\pi}{3\sqrt{3}}\,\Gamma\left(\frac{2}{3}\right)^{-6} = \frac{\sqrt{3}}{\pi} W_3(-1) \approx 0.494233 < \frac{1}{2}$
- Empirically, quite marvelously, we found — and proved by a subtle use of distributional Mellin transforms — that on $[0,2]$ as well:

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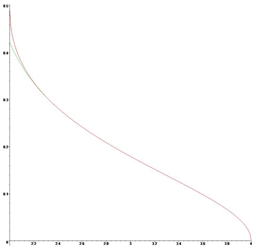

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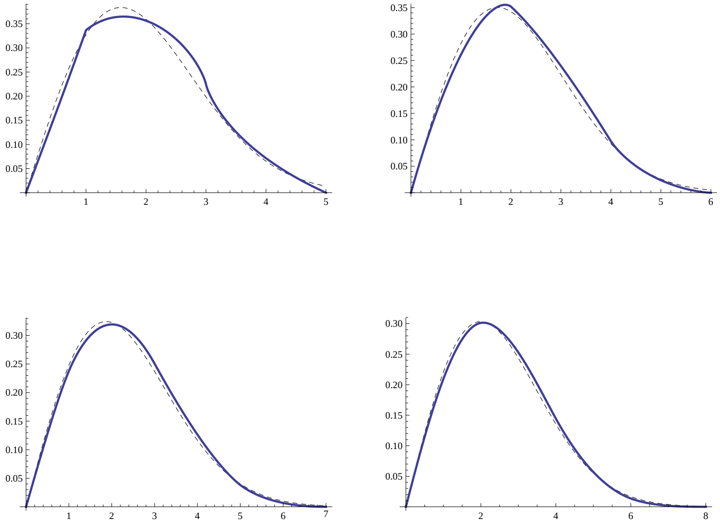
(Discovering this $\Re$ brought us full circle.)

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



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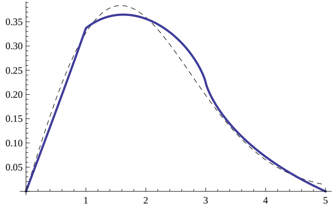
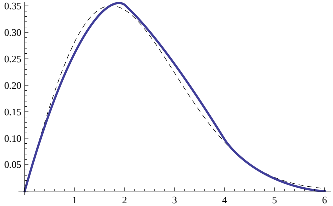
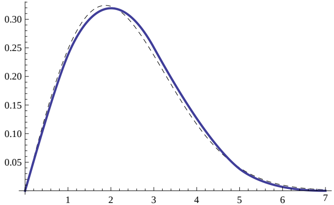
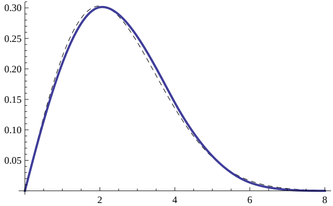




- Both p_{2n+4}, p_{2n+5} are n-times continuously differentiable for $x > 0$ $\left(p_n(x) \sim \frac{2x}{n} e^{-x^2/n}\right)$. So "four is small" *but* "eight is large."





An elliptic integral harvest

Indeed, PSLQ found various representations including:

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

$$= \frac{\pi}{4}\sum_{n=0}^{\infty} \frac{64(n+1)^4 - 144(n+1)^3 + 108(n+1)^2 - 30(n+1) + 3}{(n+1)^3}\,\frac{\binom{2n}{n}^6}{4^{6n}}.$$

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

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

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

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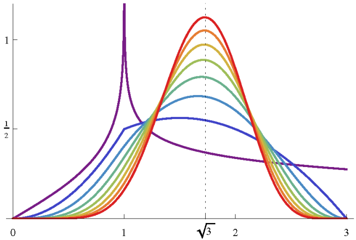
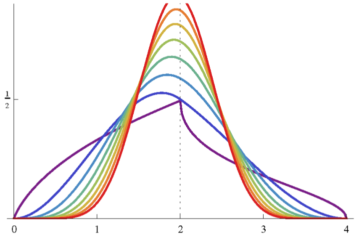
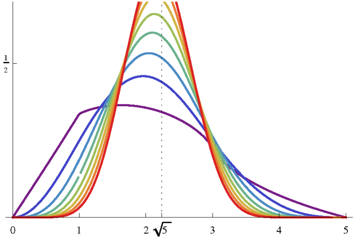
5. Four and five step densities put up more resistance!
   - and in interesting ways

V. Radial densities for $3, 4, 5$ steps in dimensions 2 to 9







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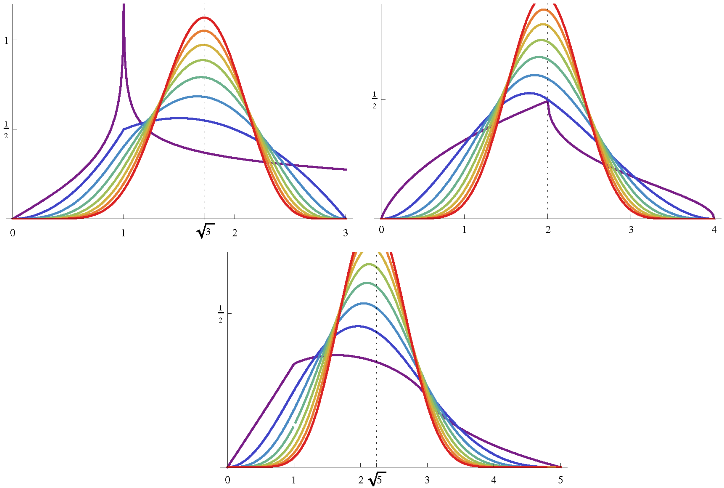

- For $x > 0$, $p_n(\nu; x)$ is m-times continuously differentiable if $m < (n-1)(\nu + 1/2) - 1$ (increases with ν and n).

Va. Even moments ... what do they count?

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Theorem (Even moments)

For all $d = 2\nu + 2$ even moments $W_n(\nu; 2k)$ are given by

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For $n = 2$ we have

$$W_2\left(\nu; 2k\right) = \frac{\binom{2(k+\nu)}{k+\nu}}{\binom{k+\nu}{\nu}}.$$

So for $\nu = 1$ and so $d = 4$, we have

$$W_2\left(1; 2k\right) = C_{k+1},$$

the Catalan number of order $k + 1$. More generally $W_n(\nu, 2k)$ is only fully integral for $\nu = 0, 1$. Indeed ...

Va. Combinatorics of even moments ... (BSV, Hare–McKay)

Theorem (BSV, 2015)

For given integer $\nu \geq 0$, let $A(\nu)$ be the infinite lower triangular matrix with entries

$$A_{k,j}(\nu) := \binom{k}{j} \frac{(k+\nu)!\nu!}{(k-j+\nu)!(j+\nu)!}$$

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- $A(1)$ is the integral Narayana triangle [A001263].

Va. Narayana Triangle

$$A(1) := \begin{bmatrix} 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \dots \\ 1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & \\ 1 & 3 & 1 & 0 & 0 & 0 & 0 & 0 & \\ 1 & 6 & 6 & 1 & 0 & 0 & 0 & 0 & \\ 1 & 10 & 20 & 10 & 1 & 0 & 0 & 0 & \\ 1 & 15 & 50 & 50 & 15 & 1 & 0 & 0 & \\ 1 & 21 & 105 & 175 & 105 & 21 & 1 & 0 & \\ 1 & 28 & 196 & 490 & 490 & 196 & 28 & 1 & \\ \vdots & & & & & & & & \ddots \end{bmatrix}$$

Va. Divisibility properties of even moments ... also congruences

For integer $\nu \geq 0$, H&M (2015) define

$$r_\nu := \min\left\{r > 0 : A_{k,j}(\nu) \in \frac{1}{r}\mathbb{Z}, j, k \geq 0\right\}.$$

so that $r_0 = r_1 = 1$ and $r_2 = 3$.

Theorem

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Conjecture (Proven for $\nu = 0, 1, 2, 3, 4$)

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Meijer-G functions (1936–)

Definition (Meijer-G)

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

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

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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.

Vb. Bessel and Meijer forms

Theorem (Meijer forms)

For all complex s, and $\nu = 0, 1/2, 1, \ldots$, with some restriction on s, we have

$$W_3(\nu; s) \quad = \quad 2^{2\nu} \nu!^2 \frac{\Gamma\left(\frac{s}{2} + \nu + 1\right)}{\Gamma\left(\frac{1}{2}\right)\Gamma\left(-\frac{s}{2}\right)} G^{2,1}_{3,3}\left(\begin{matrix} 1, 1+\nu, 1+2\nu \\ \frac{1}{2}+\nu, -\frac{s}{2}, -\frac{s}{2}-\nu \end{matrix} ; \frac{1}{4} \right),$$

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For all complex s, and $\nu = 0, 1/2, 1, \ldots$, with some restriction on s, we have

$$\begin{aligned} W_3(\nu; s) &= 2^{2\nu}\nu!^2 \frac{\Gamma\left(\frac{s}{2}+\nu+1\right)}{\Gamma\left(\frac{1}{2}\right)\Gamma\left(-\frac{s}{2}\right)} G_{3,3}^{2,1}\left(\begin{matrix} 1, 1+\nu, 1+2\nu \\ \frac{1}{2}+\nu, -\frac{s}{2}, -\frac{s}{2}-\nu \end{matrix} ; \frac{1}{4}\right), \\ W_4(\nu; s) &= 2^{s+4\nu}\nu!^3 \frac{\Gamma\left(\frac{s}{2}+\nu+1\right)}{\Gamma\left(\frac{1}{2}\right)^2 \Gamma\left(-\frac{s}{2}\right)} \\ &\times G_{4,4}^{2,2}\left(\begin{matrix} 1, \frac{1-s}{2}-\nu, 1+\nu, 1+2\nu \\ \frac{1}{2}+\nu, -\frac{s}{2}, -\frac{s}{2}-\nu, -\frac{s}{2}-2\nu \end{matrix} ; 1\right). \end{aligned}$$

Vb. Bessel and Meijer forms

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- These can be written in terms of hypergeometric functions; in the limit for odd integers.

Vc. Density in odd dimensions ... and hence also moments

Theorem (Convolution for density in odd dim., García-Pelayo 2012)

Assume the dimension $d = 2m + 1$ is odd. Then, for all real x,

$$p_n(m - 1/2; x) = \frac{(2x)^{2m}\Gamma(m)}{\Gamma(2m)} \left(-\frac{1}{2x}\frac{\mathrm{d}}{\mathrm{d}x}\right)^m P_{m,n}(x) \qquad (13)$$

where $P_{m,n}$ is the piecewise polynomial obtained from convolving

$$f_m(x) := \frac{\Gamma(m + 1/2)}{\Gamma(1/2)\Gamma(m)} \begin{cases} (1 - x^2)^{m-1} & \text{if } x \in [-1, 1] \\ 0 & \text{otherwise} \end{cases}$$

$n - 1$ times with itself.

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$n-1$ *times with itself.*

- The expression above is both elegant and compact. It shows that in odd dimensions the density is piecewise polynomial, but is difficult to manipulate or compute with or without a CAS. It leads to ...

Vc. Density in odd dimensions ... Rayleigh (1919) in 3-space

Theorem (Densities in odd dimensions, B–Sinnamon 2015)

Let $n \geq 2$ and $m \geq 1$. Then

$$p_n(m-1/2;x) = \left(\frac{\Gamma(2m)}{2^m\Gamma(m)}\right)^n \sum_{r=0}^{n} \binom{n}{r} (-1)^{mr} H(n-2r+x)$$
$$\times \sum_{k=1}^{m} (-2)^k \binom{m-1}{k-1} \frac{(2m-1-k)!}{(2m-1)!} x^k$$
$$\times \sum_{j=0}^{(m-1)n} \frac{(n-2r+x)^{mn-1+j-k}}{(mn-1+j-k)!} [x^j] C_m(x)^r C_m(-x)^{n-r} \qquad (14)$$

where $H(x)$ is the Heaviside function and

$$C_m(x) := \sum_{k=0}^{m-1} \frac{(m-1+k)!}{2^k k!(m-1-k)!} x^k = {}_2F_0\left(m, 1-m; \ ; -\frac{x}{2}\right).$$

Vd. Moments of a three step walk in even dimensions

Theorem (Three step moments)

For all integers ν and n we have

$$W_3(\nu,n) = \operatorname{Re} {}_3F_2\left(\begin{matrix}\nu+\frac{1}{2}, -n, -n-\nu \\ \nu+1, 2\nu+1\end{matrix}\,\middle|\, 4\right),$$

and, all these lie in the vector space over $\mathbb{Q}$ generated by

$$A := \frac{3}{16}\frac{2^{1/3}}{\pi^4}\Gamma^6\left(\frac{1}{3}\right) \quad \text{and} \quad \frac{1}{\pi^2 A}.$$

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This relies on discovery that

$$W_3\,(\nu; 2\,n-1) = 2\nu^2\,\frac{W_3\,(\nu-1; 2\,n+3) - 3\,W_3\,(\nu-1; 2\,n+1)}{(2n+6\nu-1)(2n+1)}. \quad (15)$$

- Theorem fails in odd dim but (15) has a partner for $n=4$ yielding all odd moments of 4-step walks in even dimensions.

Vd. Moments of a three step walk in even dimensions

Theorem (OGF for even moments with 3 steps)

For integers $\nu \geq 0$ we have

$$\sum_{k=0}^{\infty} W_3(\nu; 2k) x^k = \frac{(-1)^\nu}{\binom{2\nu}{\nu}} \frac{(1-1/x)^{2\nu}}{1+3x} {}_2F_1\left(\left.{\frac{1}{3}, \frac{2}{3} \atop 1+\nu}\right| \frac{27x(1-x)^2}{(1+3x)^3}\right) - q_\nu\left(\frac{1}{x}\right), \tag{16}$$

for $|x| < 1/9$, where $q_\nu(x)$ is a polynomial (that is, $q_\nu(1/x)$ is the principal part of the hypergeometric term on the right-hand side).

Vd. Moments of a three step walk in even dimensions

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- $q_0(x) = 0$ and $q_1(x) = \frac{1}{2x^2} - \frac{1}{x}$, etc.

Vd. Density of a three step walk in all dimensions

Theorem (Three step density)

For any half-integer ν *and* $x \in (0,3)$*, we have*

$$\frac{p_3(\nu;x)}{x} = \frac{2\sqrt{3}}{\pi} \frac{3^{-3\nu}}{\binom{2\nu}{\nu}} \frac{x^{2\nu}(9-x^2)^{2\nu}}{3+x^2} {}_2F_1\left({\frac{1}{3}, \frac{2}{3} \atop 1+\nu} ; \frac{x^2(9-x^2)^2}{(3+x^2)^3} \right). \quad (17)$$

In addition, $p_3(\nu;x)/x$ *satisfies the functional equation*

$$F(x) = \left(\frac{1+x}{2}\right)^{6\nu+2} F\left(\frac{3-x}{1+x}\right).$$

found symbolically in odd dimensions.

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General results for all $n = 3,4,5\ldots$ and $\nu > 0$ include :

$$p_{n+1}^{(d-1)}(\nu;0) = (d-1)!\,p_n(\nu;1),$$

$$p'_n(\nu;1) = \frac{(2n)\,\nu+n-1}{n+1}\,p_n(\nu;1).$$

Ve. Generalised Domb numbers ...and an OGF for (19)

We can prove $W_4(\nu; 2k) =$

$$2^{2(\nu+k)} \frac{\Gamma\left(k+\nu+\frac{1}{2}\right)\Gamma\left(1+\nu\right)}{\sqrt{\pi}\Gamma\left(1+k+2\,\nu\right)} {}_3F_2\left(\left.{-k, -k-\nu, -k-2\nu, \frac{1}{2}+\nu \atop 1+\nu, 1+2\nu, \frac{1}{2}-k-\nu}\right| 1\right). \tag{18}$$

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The Domb or *diamond lattice numbers* start: $1, 4, 28, 256, 2716, 31504, 387136, 4951552\ldots$. They are `A002895` in the OEIS with ogf

$$1+4\,x^2+28\,x^4+\ldots = \frac{1}{1-4\,x}{}_2F_1\left(\left.{\frac{1}{6}, \frac{1}{3} \atop 1}\right|\frac{108\,x^2}{(1-4\,x)^3}\right)^2.$$

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- For 4-steps in $d = 4, 6$ dim. (18) gives [A253095, 14-06-15]

$$1, 4, 22, 148, 1144, 9784, 90346, 885868, 9115276, \ldots \tag{19}$$

$$1, 4, 20, \frac{352}{3}, \frac{2330}{3}, \frac{16952}{3}, \frac{133084}{3}, 370752, 3265208, \ldots \tag{20}$$

which is what the Narayana analysis showed.

Ve. Generalised Domb numbers ...and an ogf for (19)

It was known that

$$\sum_{k=0}^{\infty} W_4(0;2k)x^k = \frac{1}{1-16x}\,{}_2F_1\left(\begin{matrix}\frac{1}{6},\frac{1}{3}\\ 1\end{matrix}\middle|\frac{108x}{(16x-1)^3}\right)^2. \tag{21}$$

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We derived, as in (16), that

$$-\frac{1}{2x^2}+\frac{1}{x}+\sum_{n=0}^{\infty} W_4(1;2k)x^k \qquad (22)$$

$$= (32x-7)F_0^2-(4x-1)\left[(32x+3)F_0F_1-\left(16x^2+10x+\frac{1}{4}\right)F_1^2\right].$$

Here, we employ hypergeometrics:

$$F_\lambda := \frac{1}{2\cdot 3^\lambda x(16x-1)^{1-\lambda}}\frac{\mathrm{d}^\lambda}{\mathrm{d}x^\lambda}\,{}_2F_1\left(\left.{\frac{1}{6},\frac{1}{3} \atop 1}\right|\frac{108x}{(16x-1)^3}\right).$$

Vf. Five step walks

... now extended to all dimensions

- The functional equation for $W_5 = W_5(0;\cdot)$ is:

$$\begin{aligned} & 225(s+4)^2(s+2)^2 W_5(s) = -(35(s+5)^4 + 42(s+5)^2 + 3)W_5(s+4) \\ + \quad & (s+6)^4 W_5(s+6) + (s+4)^2(259(s+4)^2 + 104)W_5(s+2). \end{aligned} \tag{23}$$

Q. Is there a hyper-closed form for $W_5(\mp 1)$ **?**

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- We deduce *the first two poles* — and so all — *are simple* since

$$\lim_{s\to-2}(s+2)^2 W_5(s) = \frac{4}{225}\left(285\, W_5(0) - 201\, W_5(2) + 16\, W_5(4)\right) = 0$$

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- We *stumbled* upon a proof, via Chowla-Selberg, that

$$r_{5,0} = p_4(1) = \mathrm{Res}_{-2}(W_5) = \frac{\sqrt{15}}{3\,\pi}\, {}_3F_2\left(\left.{\frac{1}{3},\frac{2}{3},\frac{1}{2} \atop 1,1}\right| -4\right).$$

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- And, originally numerically, but now proven using $\nu = 1$, that

$$r_{5,1} := \mathrm{Res}_{-4}(W_5) = \frac{13}{225} r_5(1) - \frac{2}{5\pi^4}\frac{1}{r_5(1)}.$$

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Vf. Five step walks ... now extended to all dimensions

- The functional equation for $W_5 = W_5(0;\cdot)$ is:

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Q. Is there a hyper-closed form for $W_5(\mp1)$ **?**

Vf. Five step walks

... now extended to all dimensions

We obtain three differential relations for p_5. Assisted by Koutschan's `HolonomicFunctions` package, we computed a Gröbner basis for the ideal that they generate. From that, we find there exists, in analogy with four steps, a relation

$$x^2 p_5(\nu+1;x) = A p_5(\nu;x) + B p_5'(\nu;x) + C p_5''(\nu;x) + D p_5'''(\nu;x),$$

with A, B, C, D polynomials of degrees $12, 13, 14, 15$ in x (with coefficients that are rational functions in ν).

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- We conclude inductively that, for integers ν, the density $p_5(\nu;x)$ has a Taylor expansion at $x=0$ whose Taylor coefficients are recursively computable and lie in the $\mathbb{Q}$-span of

$$r_{5,0} = \frac{\sqrt{5}}{40\pi^4}\Gamma\left(\frac{1}{15}\right)\Gamma\left(\frac{2}{15}\right)\Gamma\left(\frac{4}{15}\right)\Gamma\left(\frac{8}{15}\right)$$

  and $1/(\pi^4 r_{5,0})$.

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  and $1/(\pi^4 r_{5,0})$.
- It remains an open challenge, including in the planar case, to obtain a more explicit description of $p_5(\nu;x)$.

Vf. Five step walks ... Pearson explained

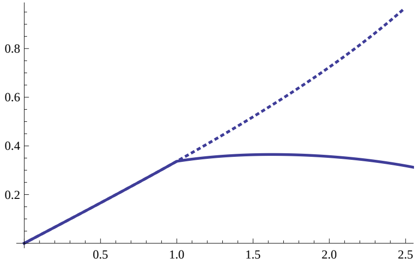

Figure: The series (dotted) and $p_5(0;x)$.

The poles of W_5 are simple, so no logarithmic terms are involved in $p_5(\nu,x)$. Computing a few more residues from the recursion (23), near 0 we have

$$p_5(0;x) = 0.329934\,x + 0.006616\,x^3 + 0.00026\,x^5 + 0.000014\,x^7 + O(x^9)$$

(with each coefficient given to six digits of precision only), explaining the strikingly straight shape of $p_5(0;x)$ on $[0,1]$.

VI. 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

$$\mu\left(1 + \sum_{k=1}^{n-1} x_k\right) = W_n'(\mathbf{0}). \tag{24}$$

which we have evaluated in for $n = 3$ and $n = 4$ respectively in terms of log-sine integrals.

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- $\mu(P)$ 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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which we have evaluated in for $n = 3$ and $n = 4$ respectively in terms of log-sine integrals.

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

Open problems (Mahler measures, II)

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

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  - Similarly for (24) $(n=5,6)$ conjectures of Villegas become:

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

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

using Dedekind's η: $\eta(q) := q^{1/24} \sum_{n=-\infty}^{\infty} (-1)^n q^{n(3n+1)/2}$.

Thank you ...

My younger collaborators (2010)

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

My younger collaborators (2010)