Densities of Short Random Walks

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Outline

I. INTRODUCTION

- An age old question: What is a walk?

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- Also random walks, random migrations, random flights.

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- I present recent results on the densities, p_n, of n-step random uniform random walks in the plane.
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- 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

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

- 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-dimensional integrals.

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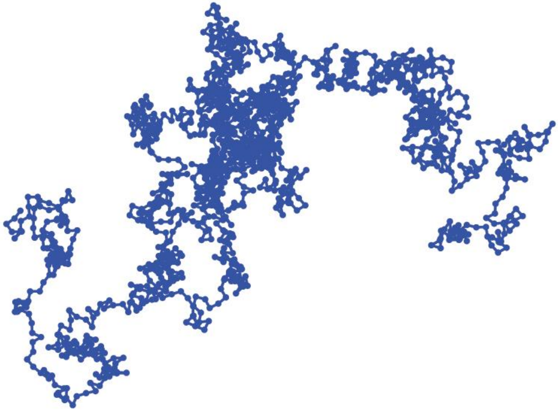
When the facts change, I change my mind. What do you do, sir?
— John Maynard Keynes in *Economist* Dec 18, 1999.

One 1500-step ramble: a familiar picture



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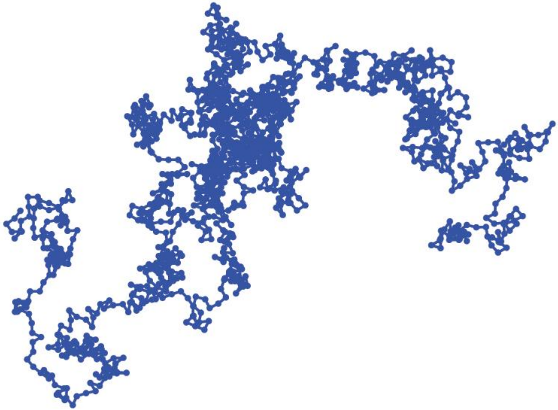

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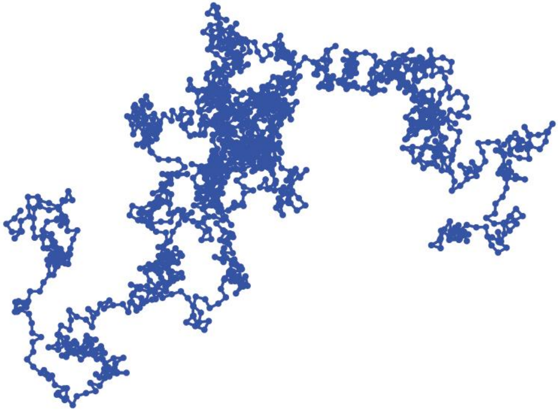
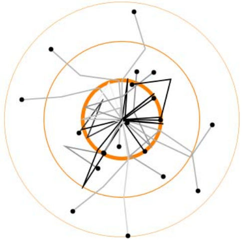


- 1D (and 3D) easy. Expectation of RMS distance is easy ($\sqrt{n}$).
- 1D or 2D *lattice*: probability one of returning to the origin.

1000 three-step rambles: a less familiar picture?



A little history — from a vast literature

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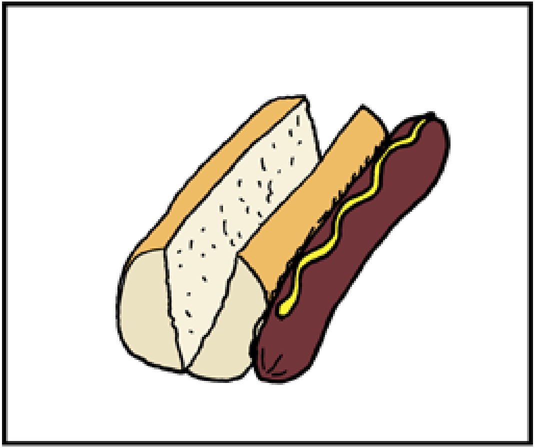
- **UNSW**: Donovan and Nuyens, WWII cryptography.
- Appear in quantum chemistry, in quantum physics as hexagonal and diamond lattice integers, etc ...

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 *OIES* 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
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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:

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

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

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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 satisfies an $\left\lfloor \frac{n+1}{2} \right\rfloor$-term recursion and $\left\lfloor \frac{n+3}{2} \right\rfloor$ distinct iterated sums:

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

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

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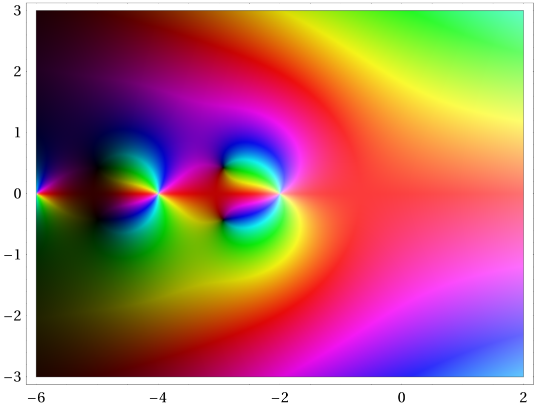
- Quasi-Monte Carlo was *not* very accurate.

III. ANALYSIS

Visualizing W_4 in the complex plane



Carlson's theorem: from discrete to continuous

Theorem (Carlson (1914, PhD))

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

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

then $f(z) = 0$ identically.

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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

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

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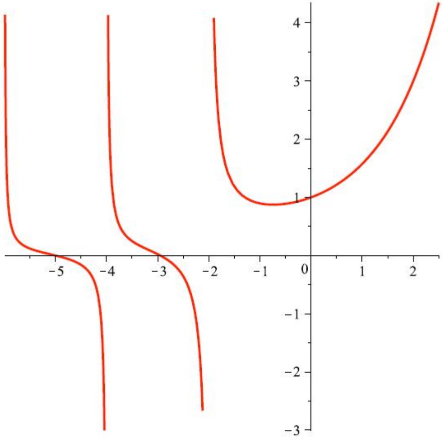
$W_3(s)$ on $[-6, \frac{5}{2}]$



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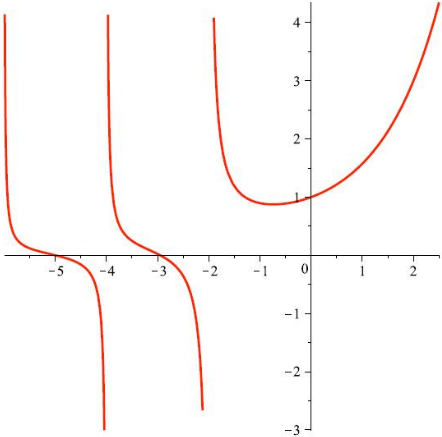

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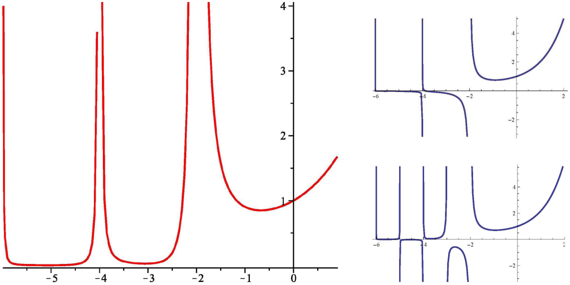
Some even dimensions look more like 4



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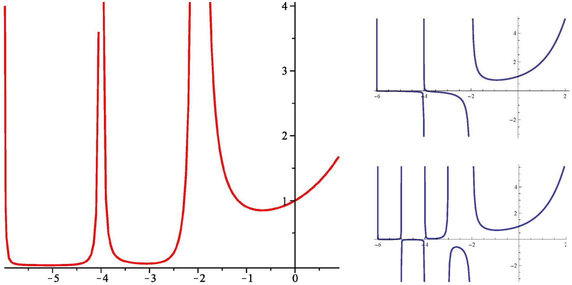

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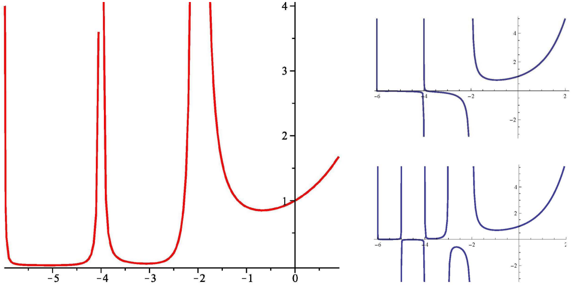

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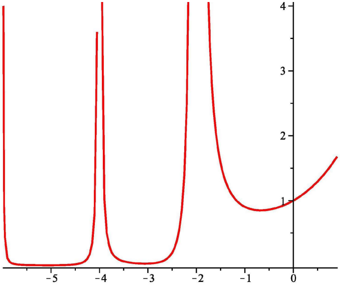

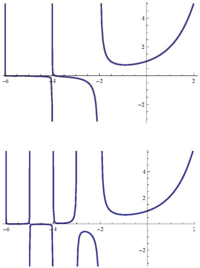

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- There are (infinitely many) multiple poles if and only if $4|n$.
- Why is W_4 positive on $\mathbf{R}$?

A discovery demystified

In particular, we had shown that

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

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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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

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

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

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

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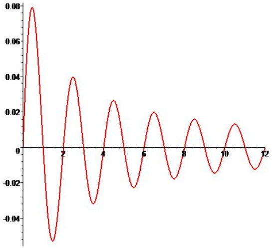
- As both sides satisfy the same 2-term recursion (computer provable), we are done. **QED**

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

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



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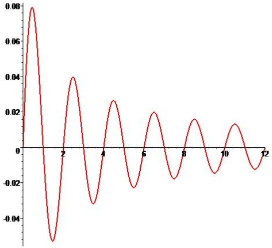

- This was hard to draw when discovered, as at the time we had no good closed form for W_3. For $s \neq -3, -5, -7, \ldots$, we now have

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

Closed forms

- We then *confirmed* 175 digits of

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

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

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.

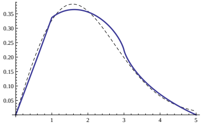
IV. PROBABILITY

It can be readily shown that

$$P_n(r) = \int_0^\infty r\, J_1(ry)\, [J_0(y)]^n\, dy \qquad (1.2)$$

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.



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:

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

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

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

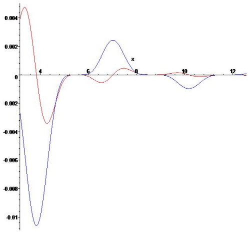
- From (6) below, we find

$$p_n(1) = \mathrm{Res}_{-2}\left(W_{n+1}\right) \qquad (n = 1, 2, \ldots). \tag{5}$$

- 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*:

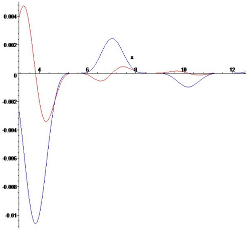
```
R:=identify(evalf[20](int(BesselJ(0,x)^3*x,x=0..infinity)))
```

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).



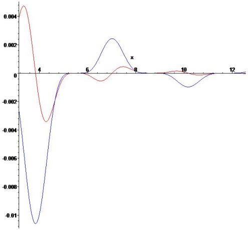
A Bessel integral for W_n

- Also $P_n(1) = \frac{J_0(0)^{n+1}}{n+1} = \frac{1}{n+1}$ (Pearson's original question).
- Broadhurst used (4) to show for $2k > s > -\frac{n}{2}$ that

$$W_n(s) = 2^{s+1-k}\frac{\Gamma(1+\frac{s}{2})}{\Gamma(k-\frac{s}{2})}\int_0^\infty x^{2k-s-1}\left(-\frac{1}{x}\frac{\mathrm{d}}{\mathrm{d}x}\right)^k J_0^n(x)\mathrm{d}x, \tag{6}$$

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

$$W_n(-1) = \int_0^\infty J_0^n(x)\mathrm{d}x, \;\; W_n(1) = n\int_0^\infty J_1(x)J_0(x)^{n-1}\frac{\mathrm{d}x}{x}. \tag{7}$$



Integrands for $W_4(-1)$ (blue) and $W_4(1)$ (red) on $[\pi, 4\pi]$ from (7).

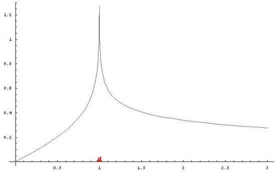
The densities for $n = 3, 4$ are modular

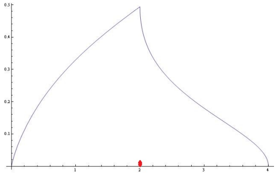
Let $\sigma(x) := \frac{3-x}{1+x}$. Then σ is an involution on $[0,3]$ sending $[0,1]$ to $[1,3]$:

$$p_3(x) = \frac{4x}{(3-x)(x+1)}\, p_3(\sigma(x)). \tag{8}$$

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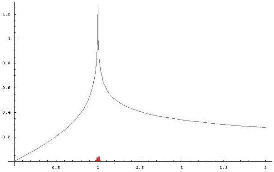
$$p_3(\alpha) = \frac{2\sqrt{3}\alpha}{\pi\ (3+\alpha^2)}\ {}_2F_1\left(\begin{matrix}\frac{1}{3}, \frac{2}{3} \\ 1\end{matrix}\,\middle|\, \frac{\alpha^2\left(9-\alpha^2\right)^2}{\left(3+\alpha^2\right)^3}\right) = \frac{2\sqrt{3}}{\pi}\, \frac{\alpha}{\mathrm{AG}_3(3+\alpha^2, 3\left(1-\alpha^2\right)^{2/3})}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

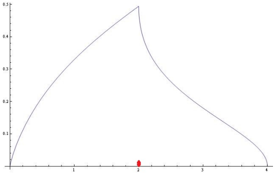
where AG_3 is the *cubically convergent* mean iteration (1991):

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

.

The densities p_3 (L) and p_4 (R)

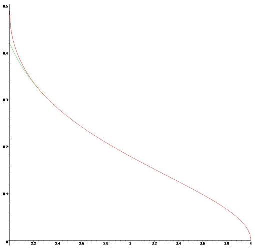




Formula for the ‘shark-fin’ p_4 (stimulated by S. Robins)

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

$$p_4(\alpha) = \frac{2}{\pi^2} \frac{\sqrt{16-\alpha^2}}{\alpha}\, {}_3F_2\left({{\frac{1}{2}, \frac{1}{2}, \frac{1}{2}} \atop {\frac{5}{6}, \frac{7}{6}}} \middle| \frac{\left(16-\alpha^2\right)^3}{108\,\alpha^4} \right). \qquad (10)$$



- ← p_4 from (10) 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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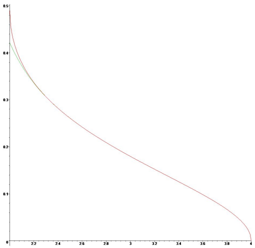

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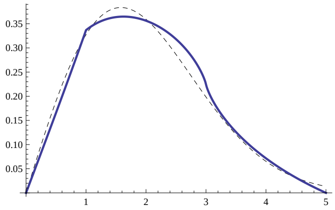
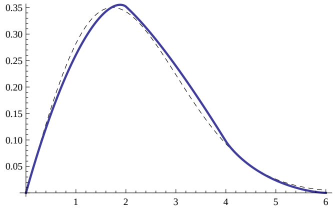
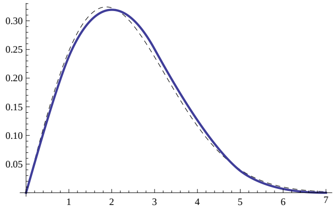
$$p_4(\alpha) \overset{?}{=} \frac{2}{\pi^2}\,\frac{\sqrt{16-\alpha^2}}{\alpha}\,\Re\;{}_3F_2\left(\left.{\frac{1}{2},\frac{1}{2},\frac{1}{2} \atop \frac{5}{6},\frac{7}{6}}\right|\frac{\left(16-\alpha^2\right)^3}{108\,\alpha^4}\right) \tag{11}$$

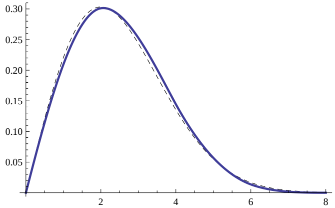
(Discovering this $\Re$ brought us full circle.)

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

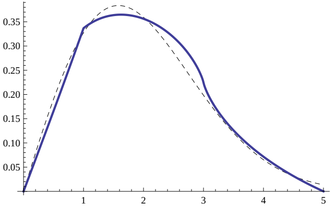


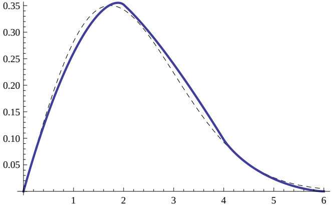




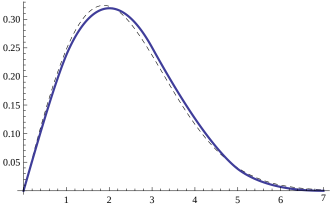


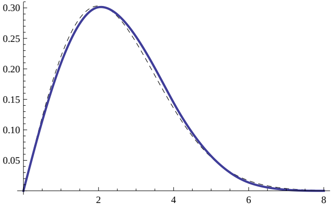
The densities for $5 \le n \le 8$ (and large n approximation)





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





An elliptic integral harvest

Indeed, PSLQ found various representations including:

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

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

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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)

V. 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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- $\mu(P)$ 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.

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- $\mu(1+x+y) = L_3'(-1) = \frac{1}{\pi}\,\mathrm{Cl}\left(\frac{\pi}{3}\right)$ (Smyth).
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  - Similarly for (12) $(n=5,6)$ 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 $\eta(q) := q^{1/24}\sum_{n=-\infty}^{\infty}(-1)^n q^{n(3n+1)/4}$.

Open problems ($n = 5$)

- The functional equation for W_5 is:

$$
\begin{aligned}
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Thank you ...

My younger collaborators

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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.

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