Random Walk Integrals

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Outline

The random walk integrals

Definition

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

Also, let $W_n := W_n(1)$.

Simplest case:

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

- 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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- 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 $W_2 = \frac{4}{\pi}$.

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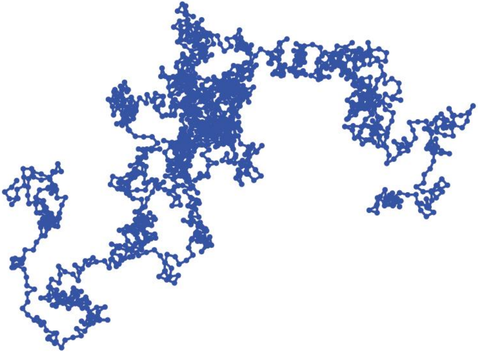
"Exactly what is a Hilbert space?" — David Hilbert

Expectations of random walk

- At each step, a unit step is taken in a random direction in the plane.
- W_n is the expected distance from the origin after n steps.
- $W_n(s)$ is the s-th moment.

Previous page: 1000 3-step walks

Below: a 1500-step walk



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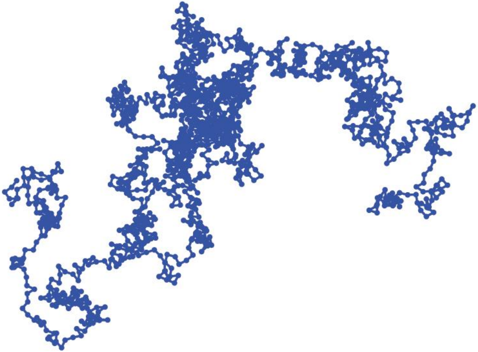

1D (and 3D) easy. Expectation of RMS distance easy ($= \sqrt{n}$).
On a lattice, has probability 1 of returning to the origin.

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- UNSW: Donovan and Nuyens, WWII cryptography.
- Also appear in quantum chemistry, in physics as hexagonal and diamond lattice integers.
- Sparked interest: Crandall, Bailey, Broadhurst, Guttmann, Zudilin, et al. Hopefully more papers to come.

Table of values

Even values are easier (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

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- Observe that $W_2(s) = \binom{s}{s/2}$ for $s > -1$.
- *MathWorld* gives $W_n(2) = n$ (trivial).

Resolution at even values

- General formula:

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

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

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- and recursion:

$$\begin{aligned}(k+2)^2 W_3(2k+4) - (10k^2+30k+23) W_3(2k+2) \\ +9(k+1)^2 W_3(2k) &= 0.\end{aligned}$$

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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$$W_n(s) = n^s \sum_{m \geqslant 0} \frac{(-1)^m}{n^{2m}} \binom{\frac{s}{2}}{m} \underbrace{\int_{[0,1]^n} \left(4 \sum_{i<j} \sin^2(\pi(x_j - x_i)) \right)^m \mathrm{d}\boldsymbol{x}}_{=: I_{n,m}}$$

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- Experimentally found recursion for $I_{3,m}$.

Conjecture. . .

- Looking up $I_{3,m}$ on Sloane: get **A093388**

$$1, 6, 42, 312, 2394, 18756, 149136, \ldots$$

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- Find that $I_{3,m}$ is coefficient of $(xyz)^m$ in

$$\begin{aligned} & (8xyz - (x+y)(y+z)(z+x))^m \\ = \quad & \left(3^2 xyz - (x+y+z)(xy+yz+zx)\right)^m \end{aligned}$$

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- Guess that $I_{n,m}$ is constant term of

$$\left(n^2 - (x_1 + \ldots + x_n)(1/x_1 + \ldots + 1/x_n)\right)^m$$

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- Leads to the conjecture

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

. . . and proof

- Need $I_{n,m} = \int_{[0,1]^n} \left(4 \sum_{i<j} \sin^2(\pi(x_j - x_i))\right)^m \mathrm{d}\boldsymbol{x}$ as the constant term of

$$\left(n^2 - (x_1 + \ldots + x_n)(1/x_1 + \ldots + 1/x_n)\right)^m =$$

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- Note that to preserve symmetry, we did not use the dimension reduction.
- Now expand the m-th power on both sides, and amazingly corresponding terms equal.

- So W_n can be evaluated in $[\frac{n+3}{2}]$ 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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- Recursion gives better approximations than many methods of numerical integration.
- Tanh-sinh quadrature works well for W_3 but not so good for $W_4 \approx 1.79909248$. Quasi-Monte Carlo not very accurate.

Binomial Transform

Binomial transform gives proof for even s.

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

$$a_n = \sum_{k=0}^{n} (-1)^k \binom{n}{k} s_k.$$

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Carlson's theorem

Theorem (Carlson)

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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- $\sin(\pi z)$ does not satisfy the conditions of the theorem, as it grows like $e^{\pi y}$ on the imaginary axis.
- $W_n(s)$ satisfies the conditions of the theorem (in fact analytic for $\Re(s) > -2$ when $n > 2$).

Analytic continuation

- So recurrence becomes functional equation, e.g.

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

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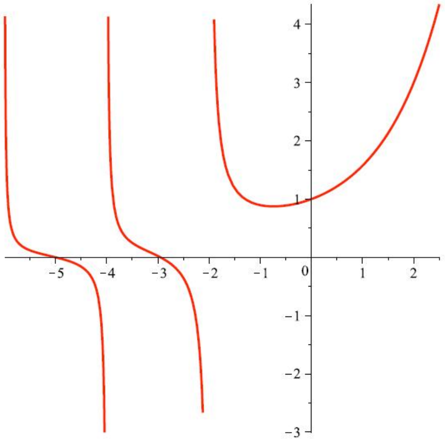
- $W_3(s)$ has a simple pole at -2 with residue $\frac{2}{\sqrt{3}\pi}$. Other simple poles at $-2k$ with residues a rational multiple of Res_{-2}.
- This gives us a "fractional binomial transform", that is, the transform gives us back a sequence that satisfies the same functional equation.

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

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



Mystery

We have

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

Here ${}_pF_q$ is the hypergeometric function.

Theorem

For integers $k \geq -1$, $W_3(k) = \Re(V_3(k))$.

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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

Hindsight proof

From the dimension reduction, and elementary manipulations,

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

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Let $s + t/2 \to s$, and using periodicity of the integrand, we end up with

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

The s integral can now be computed because

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

Here $E(x)$ is the elliptic integral of the first 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 apply Jacobi's imaginary transform,

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

where $K(x)$ is the elliptic integral of the second kind.

Using the integral definition of K and E, we write W_3 as a double integral involving only sine:

$$W_3 = \Re\left(\frac{4}{\pi^2}\int_0^{\pi/2}\int_0^{\pi/2}\frac{1+a^2\sin^2(t)-2\,a^2\sin^2(t)\sin^2(r)}{\sqrt{1-a^2\sin^2(t)\sin^2(r)}}\,\mathrm{d}t\mathrm{d}r\right),$$

where $a = 2$.

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Expand using the binomial theorem, evaluate the integral term by term for small a, and use analytic continuation to deduce equality. Similar (and easier) proof for $W_3(-1)$.

Using the integral definition of K and E, we write W_3 as a double integral involving only sine:

$$W_3 = \Re\left(\frac{4}{\pi^2}\int_0^{\pi/2}\int_0^{\pi/2}\frac{1+a^2\sin^2(t)-2\,a^2\sin^2(t)\sin^2(r)}{\sqrt{1-a^2\sin^2(t)\sin^2(r)}}\,\mathrm{d}t\mathrm{d}r\right),$$

where $a=2$.

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Similar (and easier) proof for $W_3(-1)$.
As both sides satisfy the same recursion (computer proof), we are done.

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

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- Obtained via singular values of the elliptic integral and Legendre's identity. $W_3(1)$ can be written in terms of $W_3(-1)$.

Meijer-G functions

Definition

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

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

(The contour L lies between the poles of $\Gamma(1 - a_i - s)$ and the poles of $\Gamma(b_i + s)$.)

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$W_3(s)$ is the first non-trivial higher order Meijer-G function in close form.

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

Alternative representations

- Kluyver (1906) gave a representation for the cumulative distribution function of the distance:

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

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- From this we obtain:

$$W_n(s) = \frac{(2n)^{s+2}}{s+2} \int_0^\infty {}_1F_2\left({1+\frac{s}{2} \atop 2+\frac{s}{2}, 1} \middle| -(nx)^2 \right) x\, J_0^n(x)\, \mathrm{d}x.$$

This is a 1-dimensional integral!

Simplifying the integral

- We (humans and computers) obtained:

$$
\begin{aligned}
W_4(s) &= \frac{1}{2^{2s}} \tan\left(\frac{\pi s}{2}\right) \binom{s}{\frac{s-1}{2}}^3 {}_4F_3\left(\left.\begin{matrix}\frac{1}{2}, \frac{1}{2}, \frac{1}{2}, \frac{s}{2}+1 \\ \frac{s+3}{2}, \frac{s+3}{2}, \frac{s+3}{2}\end{matrix}\right| 1\right) \\
&+ \binom{s}{\frac{s}{2}} {}_4F_3\left(\left.\begin{matrix}\frac{1}{2}, -\frac{s}{2}, -\frac{s}{2}, -\frac{s}{2} \\ 1, 1, -\frac{s-1}{2}\end{matrix}\right| 1\right).
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  Very close to a closed form.

- Turns out -1 is often easier, e.g.

$$W_4(-1) = \int_0^\infty J_0^4(x)\mathrm{d}x,$$

  CAS converts it into a Meijer-G function (in fact, now a ${}_7F_6$).

Asymptotics

- From Bessel functions, we obtain the first order approximation:

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- and second order approximation:

$$W_n(s) \approx n^{s/2-1}\left((n-\frac{1}{2})\Gamma(\frac{s}{2}+1)+\Gamma(\frac{s}{2}+2)-\frac{1}{4}\Gamma(\frac{s}{2}+3)\right),$$

in particular $W_n \approx \frac{\sqrt{n\pi}}{2}+\frac{\sqrt{\pi/n}}{32}$.

The cosine rule

- Express the distance y of an $(n+1)$-step walk conditioned on the distance x of an n-step walk by the cos rule:

$$y^2 = x^2 + 1 + 2x\cos(t).$$

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- This representation gives better insight both numerically and analytically.
- Works even better when we consider an $(n+2)$-step walk conditioned on an n step walk!

Open problems

- We have

$$W_4(2k) = \sum_{a_1+\cdots+a_4=k} \binom{k}{a_1,\ldots,a_4}^2 = \underbrace{\sum_{j\geq 0} \binom{k}{j}^2 {}_3F_2\left({{1/2, -k+j, -k+j} \atop {1,1}} \middle| 4 \right)}_{=:V_4(2k)}.$$

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Conjecture

For integers k,

$$W_4(k) = \Re(V_4(k)).$$

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Interesting blend of combinatorics, analysis, probability, and DE, all tied in with experimental mathematics.

Thank you!

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