

Uniform Random Walks on the Plane

A case study in experimental mathematics

James Wan

14 January, 2013



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The use of computers beyond routine simulations and calculations.

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A journal since 1992.

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Solving sudoku (Douglas-Rachford, convex optimization, 2010)

My use of Experimental Mathematics (1)

Gaussian quadrature:

Traditionally used to approximate integrals by finite sums and orthogonal polynomials.

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Computational insight: use discrete version to approximate sums; use orthogonal rational functions.

Surprisingly good for lattice sums, e.g. 1.4 digits per term for Madelung constant

$$\sum_{m,n,p} ' \frac{(-1)^{m+n+p}}{\sqrt{m^2 + n^2 + p^2}}.$$

My use of Experimental Mathematics (2)

Elliptic integrals: $K(x) = \int_0^{\pi/2} \frac{dt}{\sqrt{1-x^2 \sin^2 t}}$

$$\int_0^1 K(x)^3 dx = \frac{3\Gamma(1/4)^8}{1280\pi^2} \approx 7.090227004846.$$

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Galilean experiment: either gives us confidence in the view we are taking or rules out some possibilities.

My use of Experimental Mathematics (3)

Special functions:

Computer assisted discovery and *automatic* proof of the g.f.

$$\begin{aligned}
 & (1 - cxy) \left\{ \sum_{n=0}^{\infty} u_n x^n \right\} \left\{ \sum_{n=0}^{\infty} u_n y^n \right\} \\
 &= \sum_{n=0}^{\infty} u_n P_n \left(\frac{(x+y)(1+cxy) - 2axy}{(y-x)(1-cxy)} \right) \left(\frac{y-x}{1-cxy} \right)^n,
 \end{aligned}$$

where $(n+1)^2 u_{n+1} = (an^2 + an + b)u_n - cn^2 u_{n-1}$.

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$$\sum_{n=0}^{\infty} \left\{ \sum_{k=0}^n \sum_{j=0}^k \binom{n}{k} \left(\frac{-1}{8} \right)^k \binom{k}{j}^3 \right\} n P_n \left(\frac{5}{3\sqrt{3}} \right) \left(\frac{4}{3\sqrt{3}} \right)^n = \frac{9\sqrt{3}}{2\pi}.$$

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Very basic problem; sum of n random complex numbers.

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All our discoveries were experimental.

Hypergeometric series:

$${}_pF_q \left(\begin{matrix} a_1, \dots, a_p \\ b_1, \dots, b_q \end{matrix} \middle| z \right) = \sum_{n=0}^{\infty} \frac{(a_1)_n \cdots (a_p)_n}{(b_1)_n \cdots (b_q)_n} \frac{z^n}{n!}.$$

Random walk integrals

Definition: For complex s ,

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

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Dimension reduction: let $x_1 = 0$.

Computational challenge

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- *Maple 13* and *Mathematica 7* think $W_2 = 0$.
- $p_2(x) = \frac{2}{\pi\sqrt{4-x^2}}, W_2(s) = \binom{s}{s/2}, W_2(1) = \frac{4}{\pi}$.

Computational challenge

- $W_1(s) = 1$, $p_1(x) = \delta_1(x)$.
- *Maple 13* and *Mathematica 7* think $W_2 = 0$.
- $p_2(x) = \frac{2}{\pi\sqrt{4-x^2}}$, $W_2(s) = \binom{s}{s/2}$, $W_2(1) = \frac{4}{\pi}$.
- Tanh-sinh quadrature gives 175 digits for $W_3(1)$, but everything fails for $W_4(1)$. 256 cores at LBNL:
 $W_5(1) \approx 2.0081618$.

Jan Cornelius Kluyver & John William Strutt

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- Probability of returning to the unit disk:

$$\int_0^1 p_n(t) dt = \int_0^\infty J_1(x) J_0^n(x) dx = \left[\frac{-J_0(x)^{n+1}}{n+1} \right]_0^\infty = \frac{1}{n+1}.$$

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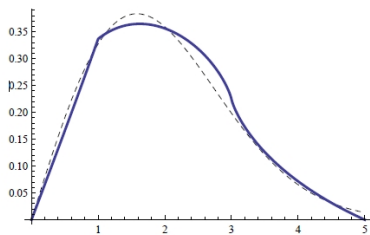
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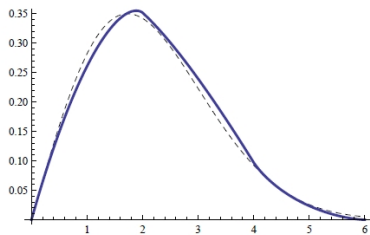
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- Rayleigh (multivariate CLT): $p_n(x) \approx \frac{2x}{n} e^{-x^2/n}.$

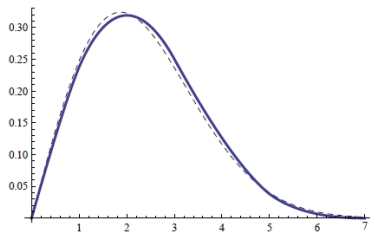
p_n with approximations superimposed.



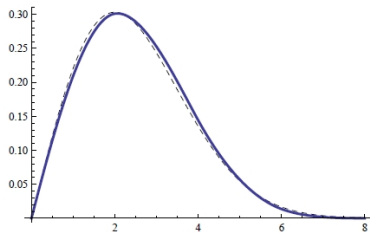
(a) p_5



(b) p_6



(c) p_7



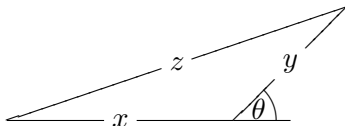
(d) p_8

Probability

- We condition the distance z of an $(n + m)$ -step walk on x (n steps), followed by y (m steps).

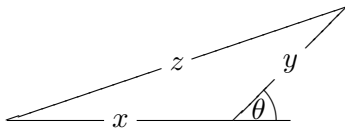
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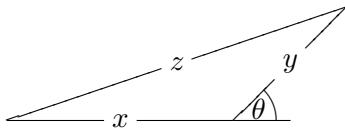
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- Change of variable:

$$W_{n+m}(s) = \int_0^{n+m} z^s \underbrace{\left\{ \int_0^n \int_0^\pi \frac{z}{\pi y} p_n(x) p_m(y) d\theta dx \right\}}_{p_{n+m}(z)} dz.$$

Recursion for p_n

- $\therefore p_n$ is a single integral over p_{n-1} . So

$$p_3(x) = \frac{2\sqrt{3}x}{\pi(3+x^2)} {}_2F_1\left(\frac{1}{3}, \frac{2}{3} \middle| \frac{x^2(9-x^2)^2}{(3+x^2)^3}\right).$$

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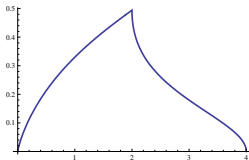
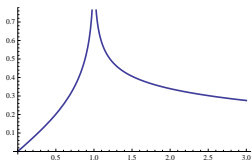
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- p_4 hard to compute; we resort to moments and analytic continuation.



Combinatorics and analysis

- Binomial expansion:

$$W_n(s) = n^s \sum_{m \geq 0} \frac{(-1)^m}{n^{2m}} \binom{\frac{s}{2}}{m} I_{n,m}.$$

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- Has a recursion \Rightarrow lifts to a functional equation $\Rightarrow W_n(s)$ has analytical continuation to \mathbb{C} with poles at negative integers.

Three steps

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Theorem (1), Borwein, Nuyens, Straub, W. (2009)

$$W_3(1) = \frac{16\sqrt[3]{4}\pi^2}{\Gamma(\frac{1}{3})^6} + \frac{3\Gamma(\frac{1}{3})^6}{8\sqrt[3]{4}\pi^4} \approx 1.57459723755.$$

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Proven using elementary manipulation of integrand and the **transform** $\operatorname{Re} K(1/x) = xK(x)$.

Four steps

Theorem (2), Borwein, Straub, W., Zudilin (2010)

$W_4(1) \approx 1.79909248$ is given by

$$\frac{3\pi}{4} {}_7F_6 \left(\begin{matrix} \frac{7}{4}, \frac{3}{2}, \frac{3}{2}, \frac{3}{2}, \frac{1}{2}, \frac{1}{2}, \frac{1}{2} \\ \frac{3}{4}, 2, 2, 2, 1, 1 \end{matrix} \middle| 1 \right) - \frac{3\pi}{8} {}_7F_6 \left(\begin{matrix} \frac{7}{4}, \frac{3}{2}, \frac{3}{2}, \frac{1}{2}, \frac{1}{2}, \frac{1}{2}, \frac{1}{2} \\ \frac{3}{4}, 2, 2, 2, 2, 1 \end{matrix} \middle| 1 \right).$$

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$$W_4(s) = \frac{2^s}{\pi^3} \frac{\Gamma(1+s/2)}{\Gamma(-s/2)} G_{4,4}^{2,4} \left(\begin{matrix} 1, (1-s)/2, 1, 1 \\ 1/2, -s/2, -s/2, -s/2 \end{matrix} \middle| 1 \right).$$

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- Split triple integral in 2, *Zudilin's theorem*: $\implies {}_7F_6$.

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- Also explains the shape of p_5 .
- If p_4 admits a Taylor series around 0, this argument would give simple poles for $W_4(s)$, but it has double poles. **!?**

Series for p_4

- Plot $p'_4(x)$ for small x was best done from *first principles*.
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- Solution: $f(x) = (a - r \log x)x$, $a \approx 0.33$, explaining the double pole!

Closed form for p_4

- To be consistent, we must have:

$$p_4(x) = \sum_{n=1}^{\infty} (a_4(n) - r_4(n) \log x) x^{2n-1},$$

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- More work on modular forms:

Theorem (3) Borwein, Straub, W., Zudilin (2010)

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

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Thank you!



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