

Self-avoiding walks in a rectangle

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- In **SIAM News, January 2002** L N Trefethen presented 10 canonical numerical analysis problems.
- The answer to each was a real number. Trefethen sought 10 sig. digits for each problem. The 100 digit challenge.
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Problem 10

A particle at the center of a 10×1 rectangle undergoes Brownian motion (i.e., two-dimensional random walk with infinitesimal step lengths) until it hits the boundary. What is the probability that it hits at one of the ends rather than at one of the sides?

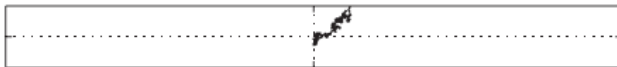


Figure 10.1. *A sample path hitting at the upper side.*

- Many attempts at solving this, including
Monte Carlo: A sample size of 10^8 gives an estimate 4×10^{-7} .
- Approximate Brownian motion by a simple random walk and make the mesh size small.
- Can be recast as discrete Laplace equation with Dirichlet boundary conditions.
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- The solution in the Brownian motion case is the *harmonic measure* of the end w.r.t the rectangular domain.
- Harmonic measure of a bounded domain in \mathbb{R}^n ($n > 1$) is the probability that a Brownian motion started inside a domain hits a portion of the boundary.
- What value does the harmonic measure of the ends of a 10×1 rectangle take at the centre?
- Can be solved by finite-difference methods and convergence acceleration. $p = 3.837587979 \times 10^{-7}$.

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HOW DOES THE HITTING DENSITY TRANSFORM?

- Let $h_D(z)$ denote the hitting density w.r.t. arc-length of the domain. (Poisson kernel).
- Let f be a conformal map on D that fixes the origin, and s.t. the boundary is piecewise smooth.
- Then conformal invariance relates the density for harmonic measure on the boundary of $f(D)$ to the boundary of D by

$$h_D(z) = |f'(z)| h_{f(D)}(f(z)).$$

- For SAW, let the corresponding probability density be $\rho(z)$. Then Lawler Schramm and Werner calculated that under a conformal map

$$\rho_D(z) = c |f'(z)|^b \rho_{f(D)}(f(z)),$$

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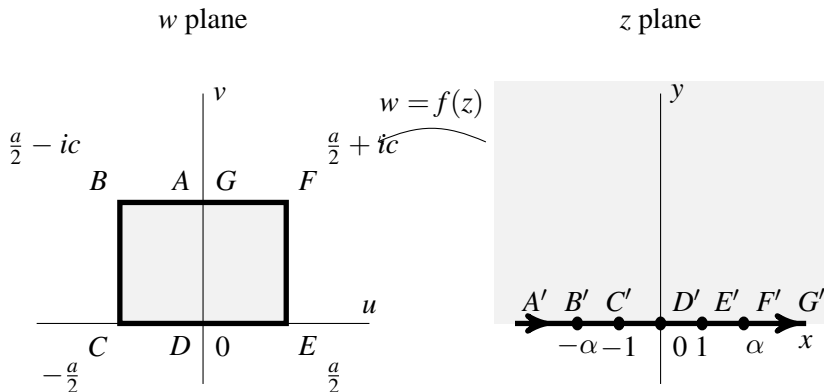
where $b = 5/8$. (More generally b is related to κ .)

- Starting at the centre of a disc, it is clear that the hitting density is uniform on the boundary.
- So these equations determine the hitting density for any simply connected domain
- For non-rectangular domains, there is a lattice effect that persists in the scaling limit – producing a factor that depends on the angle of the boundary tangent that must be included.
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Mapping of \mathbb{H} to a rectangle.
$$f(z) = \int_0^z \frac{d\xi}{\sqrt{1-\xi^2} \sqrt{\alpha^2 - \xi^2}}.$$

- The Schwarz-Christoffel transformation mapping \mathbb{H} to an $a \times c$ rectangle as shown is

$$f(z) = \int_0^z \frac{d\xi}{\sqrt{1-\xi^2}\sqrt{\alpha^2-\xi^2}}.$$

- The corners are mapped so that

$$f(1) = a/2, f(-1) = -a/2, f(\alpha) = a/2+ic, f(-\alpha) = -a/2+ic.$$

- So

$$a = \int_{-1}^1 \frac{dx}{\sqrt{1-x^2}\sqrt{\alpha^2-x^2}}, \quad c = \int_1^\alpha \frac{dx}{\sqrt{x^2-1}\sqrt{\alpha^2-x^2}}.$$

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$$a = \frac{2}{\alpha} \mathbf{K} \left(\frac{1}{\alpha} \right), \quad c = \frac{1}{\alpha} \mathbf{K} \left(\frac{\sqrt{\alpha^2-1}}{\alpha} \right) = \frac{1}{\alpha} \mathbf{K}' \left(\frac{1}{\alpha} \right), \quad \alpha > 1.$$

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- The aspect ratio $r = a/c$, so

$$r = \frac{2\mathbf{K}(1/\alpha)}{\mathbf{K}'(1/\alpha)},$$

- The nome q is defined $q = \exp(-\pi\mathbf{K}'/\mathbf{K})$
- So $e^{-2\pi/r} = q$, which can be solved to give

$$\alpha = \left(\frac{\theta_3(q)}{\theta_2(q)} \right)^2.$$

- So α can be evaluated for any $r \geq 1$ numerically. Asymptotically

$$\pi r = 4 \log(2\sqrt{2}) - 2 \log(\alpha - 1) + (\alpha - 1) - \frac{3}{8}(\alpha - 1)^2 + O(\alpha - 1)^3.$$

Solving this numerically for $r = 10$ gives

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- We need walks from the centre of the rectangle to the boundary. By symmetry, the preimage will be on the imaginary axis in \mathbb{H} . Call it id .
- From the S-C mapping $f(z) = \int_0^z \frac{d\xi}{\sqrt{1-\xi^2}\sqrt{\alpha^2-\xi^2}}$, set $u = -i\xi$, giving $ic/2 = f(id) = i \int_0^d \frac{du}{\sqrt{1+u^2}\sqrt{\alpha^2+u^2}}$.
- This integral is an (incomplete) elliptic integral of the second kind, from which we find $d = \sqrt{\alpha}$.
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CALCULATING THE HITTING DENSITY

- The hitting density for Brownian motion or the scaling limit of SAW starting at the centre of a disc is clearly uniform on the boundary.
- Take D to be \mathbb{H} and f to be the conformal map from D to the unit disc, (sending i to 0), then $\rho_{f(D)}$ is constant.
- So the exit densities are just proportional to $|f'(z)|^b$.
- But $f(z) = \frac{z-i}{z+i}$, and for z real, ($z = x$), we have $|f'(x)| = \frac{2}{x^2+1}$.
- If instead the walk starts at $z = i\sqrt{\alpha}$, (rather than $z = i$), then by scaling the hitting density is proportional to $(x^2 + \alpha)^{-b}$.

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- So the hitting density for a walk starting at the centre.

$$(x^2 + \alpha)^{-b} \propto |f'(x)|^b \rho_R(f(z)).$$

- The probability ratio $R(\alpha, b)$ is the ratio of the integral of $\rho_R(z)$ along a vertical edge to that along a horizontal edge,

$$R(\alpha, b) = \frac{\int_0^c \rho_R(a/2 + iy) dy}{\int_{-a/2}^{a/2} \rho_R(x) dx}.$$

- Set $u = f^{-1}(x)$ (denominator), $u = f^{-1}(a/2 + iy)$ (numerator),

$$R(\alpha, b) = \frac{\int_1^\alpha \rho_R(f(u)) |f'(u)| du}{\int_{-1}^1 \rho_R(f(u)) |f'(u)| du}.$$

- Recall that $f'(u) = (1 - u^2)^{-1/2}(\alpha^2 - u^2)^{-1/2}$, so

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- So the hitting density for a walk starting at the centre.

$$(x^2 + \alpha)^{-b} \propto |f'(x)|^b \rho_R(f(z)).$$

- The probability ratio $R(\alpha, b)$ is the ratio of the integral of $\rho_R(z)$ along a vertical edge to that along a horizontal edge,

$$R(\alpha, b) = \frac{\int_0^c \rho_R(a/2 + iy) dy}{\int_{-a/2}^{a/2} \rho_R(x) dx}.$$

- Set $u = f^{-1}(x)$ (denominator), $u = f^{-1}(a/2 + iy)$ (numerator),

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- These integrals can be done numerically, giving

$$R(10, 5/8) = 6.682989935 \dots \times 10^{-5},$$

some 200 times higher than for Brownian motion.

- Asymptotics is relatively straightforward for the leading term, and we find

$$\tilde{R}(r, b) \approx \frac{2^{2b} \Gamma\left(\frac{1}{2} + \frac{b}{2}\right)^2}{\Gamma\left(1 + \frac{b}{2}\right) \Gamma\left(\frac{b}{2}\right)} e^{-\pi b r / 2}.$$

- For SAW, $\tilde{R}(r, 5/8) \approx 1.2263431442 e^{-5\pi r / 16}$.
- For $r = 10$ this gives $\tilde{R}(10, 5/8) \approx 6.6824528 \times 10^{-5}$.

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$$\Lambda = \frac{\Gamma\left(\frac{1+b}{2}\right)^2}{\Gamma\left(\frac{b}{2}\right)^2}.$$

- Then $\tilde{R}(r, b) =$

$$\frac{2^{2b+1}\Lambda}{b e^{b\pi r/2}} \left[1 + \frac{\Lambda 2^{b+1} e^{-b\pi r/2}}{b \sin\left(\frac{\pi b}{2}\right)} + 4(b-1+2\Lambda)e^{-\pi r/2} + O(e^{-b\pi r}) \right],$$

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TEST THAT THE SCALING LIMIT OF SAW IS $SLE_{8/3}$.

- Enumerate all walks in a rectangle of fixed aspect ratio, as large as possible.
- Extrapolate the ratio of the (number of walks hitting the end)/(the number of walks hitting the side) for larger and larger rectangles.
- From the inverse of the above asymptotic result, determine b which is equivalent to κ . ($b = \frac{3}{\kappa} - \frac{1}{2}$.)
- We did this for walks in a rectangle of aspect ratio 2 and 10.
- We find $b = 0.624 \pm 0.002$, so that $\kappa = 2.668 \pm 0.005$.

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HITTING DENSITY DISTRIBUTION

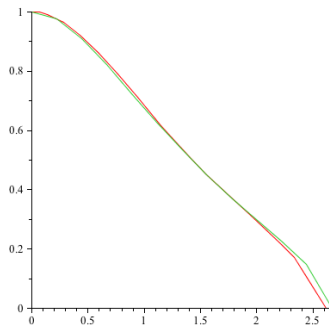


Figure: Hitting density, theoretical ($b = 5/8$) vs. that in a 14×28 rectangle.

CONCLUSION

- We can calculate the hitting ratio of paths whose scaling limit is given by SLE_κ (κ suitably restricted), in a rectangle.
- For Brownian motion ($\kappa = 2$) we can obtain the exact result, while for other values of κ we can obtain as many digits as any (reasonable) woman would wish.
- Accurate asymptotics are obtained – which can be improved.
- For the scaling limit of SAW we find the probability ratio to be some 200 times greater than that for Brownian motion.
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