Random walk with barycentric self-interaction

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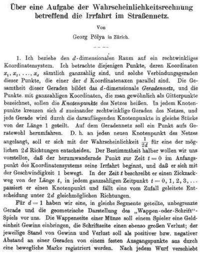
Simple random walk

Let X_n be symmetric simple random walk (SRW) on $\mathbb{Z}^d$, i.e., given $X_1, \ldots, X_n$, the new location X_{n+1} is uniformly distributed on the $2d$ adjacent lattice sites to X_n.

Theorem (Pólya 1921)

SRW is recurrent if $d = 1$ or $d = 2$, but transient if $d \geq 3$.



Über eine Aufgabe der Wahrscheinlichkeitsrechnung betreffend die Irrfahrt im Straßennetz.

Von

Georg Pólya in Zürich.

1. Ich beziehe den d-dimensionalen Raum auf ein rechtwinkliges Koordinatensystem. Ich betrachte diejenigen Punkte, deren Koordinaten $x_1, x_2, \ldots, x_d$ sämtlich ganzzahlig sind, und solche Verbindungsgeraden dieser Punkte, die einer der d Koordinatenaxen parallel sind. Die Gesamtheit dieser Geraden bildet das d-dimensionale *Geradennetz*, und die Punkte mit ganzzahligen Koordinaten, die man gewöhnlich als Gitterpunkte bezeichnet, sollen die *Knotenpunkte* des Netzes heißen. In jedem Knotenpunkte kreuzen sich d zueinander rechtwinklige Geraden des Netzes, und jede Gerade wird durch die daraufliegenden Knotenpunkte in gleiche Stücke von der Länge 1 geteilt. Auf dem Geradennetz soll ein Punkt aufs Geratewohl herumfahren. D. h. an jeden neuen Knotenpunkt des Netzes angelangt, soll er sich mit der Wahrscheinlichkeit $\frac{1}{2d}$ für eine der möglichen $2d$ Richtungen entscheiden. Der Bestimmtheit halber wollen wir uns vorstellen, daß der herumwandernde Punkt zur Zeit $t = 0$ im Anfangspunkt des Koordinatensystems seine Irrfahrt beginnt, und daß er sich mit der Geschwindigkeit 1 bewegt. In der Zeit t beschreibt er einen Zickzackweg von der Länge t, in jedem ganzzahligen Zeitpunkt $t = 0, 1, 2, 3, \ldots$ passiert er einen Knotenpunkt und fällt eine vom Zufall geleitete Entscheidung unter $2d$ gleichmöglichen Richtungen.

Für $d = 1$ haben wir eine, in gleiche Segmente geteilte, unbegrenzte Gerade und die geometrische Darstellung des „Wappen-oder-Schrift"-Spiels vor uns. Die Wappenseite einer Münze soll einem Spieler eine Geldeinheit Gewinn einbringen, die Schriftseite einen ebenso großen Verlust; der jeweilige Stand von Gewinn und Verlust soll als positiver bzw. negativer Abstand an einer Geraden von einem festen Ausgangspunkte aus durch eine bewegliche Marke registriert werden. Nach jedem Wurf verschiebt

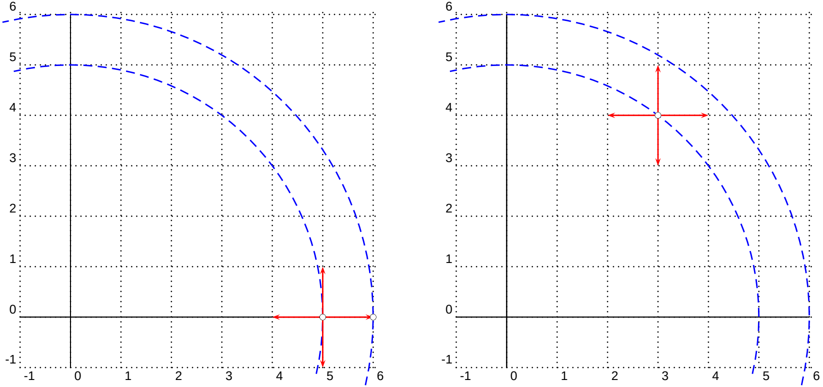
"A drunk man will find his way home, but a drunk bird may get lost forever." —Shizuo Kakutani

Lyapunov functions

- There are several proofs of Pólya's theorem available, typically using combinatorics or electrical network theory.
- These classical approaches are of limited use if one starts to generalize or perturb the model slightly.
- Lamperti (1960) gave a very robust approach, based on the method of Lyapunov functions.
- Reduce the d-dimensional problem to a 1-dimensional one by taking $Z_n := \|X_n\|$.
- $Z_n = 0$ if and only if $X_n = 0$, but the reduction of dimensionality comes at a (modest) price: Z_n is not in general a Markov process.

Lyapunov functions (cont.)

E.g. in $d = 2$, consider the two events $\{X_n = (3,4)\}$ and $\{X_n = (5,0)\}$. Both imply $Z_n = 5$, but in only one case is there positive probability of $Z_{n+1} = 6$.



So our methods cannot rely on the Markov property.

Lyapunov functions (cont.)

- Elementary calculations based on Taylor's theorem and properties of the increments $\Delta_n = X_{n+1} - X_n$ show that

$$\mathbb{E}[Z_{n+1} - Z_n \mid X_1, \ldots, X_n] = \frac{1}{2Z_n}\left(1 - \frac{1}{d}\right) + O(Z_n^{-2}),$$
$$\mathbb{E}[(Z_{n+1} - Z_n)^2 \mid X_1, \ldots, X_n] = \frac{1}{d} + O(Z_n^{-1}).$$

- In particular, Z_n is a stochastic process on $[0, \infty)$ with asymptotically zero drift.
- Loosely speaking, if $\mu_k(z) = \mathbb{E}[(Z_{n+1} - Z_n)^k \mid Z_n = z]$, we have $\mu_1(z) \sim \frac{1}{2z}\left(1 - \frac{1}{d}\right)$ and $\mu_2(z) \sim \frac{1}{d}$.

Lamperti's problem

In the early 1960s, Lamperti studied in detail how the asymptotics of a stochastic process $Z_n \in [0, \infty)$ are determined by the first two moment functions of its increments, μ_1 and μ_2.

Theorem (Lamperti 1960–63)

Under mild regularity conditions, the following recurrence classification holds.

- *If $2z\mu_1(z) - \mu_2(z) > \varepsilon > 0$, Z_n is transient.*
- *If $2z\mu_1(z) + \mu_2(z) < -\varepsilon < 0$, Z_n is positive-recurrent.*
- *If $|2z\mu_1(z)| \le \mu_2(z)$, Z_n is null-recurrent.*

Lamperti's problem (cont.)

- In particular, for $Z_n = \|X_n\|$ the norm of SRW,

$$2z\mu_1(z) \sim 1 - \frac{1}{d}, \quad \text{and} \quad \mu_2(z) \sim \frac{1}{d}.$$

  So $2z\mu_1(z) - \mu_2(z) > 0$ if and only if $d > 2$.
- So Pólya's theorem follows.
- This approach allows one to study much more general random walk models, including spatially non-homogeneous random walks, and non-Markovian processes.
- More generally, many near-critical stochastic systems, if a suitable Lyapunov function exists, can be analysed using Lamperti's theorem.

Lamperti's problem (cont.)

- An interesting family of examples is provided by centrally biased random walks.
- A concrete example: For $\mathbf{x} \in \mathbb{R}^d$, let $\mathbf{b}_1(\mathbf{x}), \ldots, \mathbf{b}_d(\mathbf{x})$ denote an orthonormal basis for $\mathbb{R}^d$ such that $\mathbf{b}_1(\mathbf{x}) = \mathbf{u}(\mathbf{x})$, where $\mathbf{u}(\mathbf{x}) := \mathbf{x}/\|\mathbf{x}\|$.
- For $i \in \{2, \ldots, d\}$, take

$$\mathbb{P}[X_{n+1} - X_n = \pm \mathbf{b}_i(X_n) \mid X_1, \ldots, X_n] = \frac{1}{2d}.$$

- Also (with an unimportant correction if $\|X_n\|$ is small) set

$$\mathbb{P}[X_{n+1} - X_n = \pm \mathbf{b}_1(X_n) \mid X_1, \ldots, X_n] = \frac{1}{2d} \pm \frac{\rho}{2}\|X_n\|^{-\beta}.$$

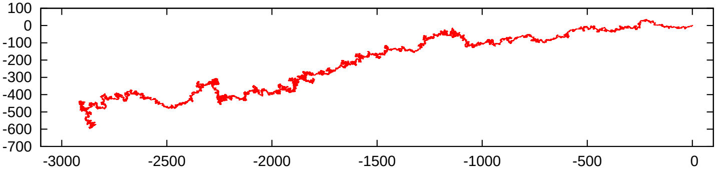
- Fixed parameters $\rho \in \mathbb{R}$ and $\beta > 0$.

Centrally biased walk

Such a model has a mean drift of the form

$$\mathbb{E}[X_{n+1} - X_n \mid X_1, \ldots, X_n] = \rho \|X_n\|^{-\beta} \mathbf{u}(X_n),$$

which is asymptotically zero as $\|X_n\| \to \infty$.



Here is a simulation of 10^5 steps of a centrally biased random walk with $\rho = 1$ and $\beta = 1/2$.

Centrally biased walk (cont.)

- Again we consider the Lyapunov function $Z_n = \|X_n\|$.
- This time

$$\mu_1(z) \sim \left(\rho + \frac{d-1}{2d}\mathbf{1}\{\beta = 1\}\right) z^{-\beta}, \text{ and } \mu_2(z) \sim \frac{1}{d}.$$

- The critical case from the point of view of recurrence/transience is when $\beta = 1$. Then $2z\mu_1(z) - \mu_2(z) \sim 2\rho + \frac{d-1}{d} - \frac{1}{d} > 0$ if $\rho > \frac{2-d}{2d}$. So, for example, if $d = 2$ the walk is transient for any $\rho > 0$.

Centrally biased walk (cont.)

- Centrally biased random walks in the critical case ($\beta = 1$) can be viewed as prototypical near-critical stochastic systems.
- They can be positive-recurrent, null-recurrent, or transient.
- But even if transient, they are diffusive,...
- and even if positive-recurrent, they do not possess geometric ergodicity: return times and stationary distributions have heavy tails.

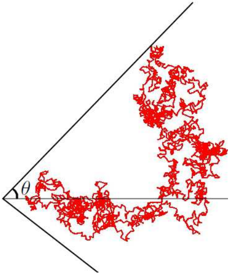
Centrally biased walk: Critical case

Theorem (Lamperti 1960–63)

Consider the centrally biased random walk in $\mathbb{R}^d$ with drift parameters $\rho \in \mathbb{R}$ and $\beta = 1$. Then, under mild conditions, the following recurrence classification holds.

- *If $\rho > \frac{2-d}{2d}$, the walk is transient.*
- *If $\rho < -\frac{1}{2}$, the walk is positive-recurrent.*
- *If $-\frac{1}{2} \leq \rho \leq \frac{2-d}{2d}$, the walk is null-recurrent.*

MMW (2010) studied the angular asymptotics of such processes, and showed, for example, that in all the cases covered by the theorem above, the walk has no limiting direction, and visits any cone infinitely often.



Centrally biased walk: Supercritical case

If $\rho > 0$ and $\beta \in (0,1)$, the walk is transient, and the rate of escape is super-diffusive but sub-ballistic, as shown by the following result.

Theorem (MMW 2009, MW 2009)

Suppose $\rho > 0$, $\beta \in (0,1)$. Then X_n is transient with a limiting direction, i.e., $\mathbf{u}(X_n) \to \mathbf{u}$ a.s. for some (random) unit vector $\mathbf{u}$. Moreover there is a law of large numbers

$$n^{-\frac{1}{1+\beta}} \|X_n\| \to \lambda(\rho, \beta) \quad (\text{constant}) \text{ a.s.}$$

In $d = 1$, there is an accompanying central limit theorem [MW 2009] which says that

$$\frac{X_n - \lambda(\rho,\beta) n^{\frac{1}{1+\beta}}}{\sqrt{n}} \to \text{normal}.$$

Polymer chains in solution

- Polymer molecules in solution are often modelled by random walks $(X_1, X_2, \dots, X_n)$ in $\mathbb{R}^d$.
- The positions X_i represent the locations of the polymer's constituent monomers, and the increment vectors $X_{i+1} - X_i$ represent the chemical bonds.
- Typically, all bonds are about the same length. To keep things simple, we work on a scale such that, for all our models, $\|X_{i+1} - X_i\| = 1$.

Polymer asymptotics

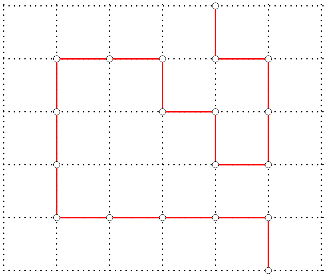
- A fundamental question is the asymptotic behaviour of the end-to-end distance $\|X_n\|$, as $n \to \infty$.
- SRW is diffusive: $\mathbb{E}\|X_n\| \approx n^{1/2}$.
- In real polymer chains, behaviour is often very different, due to:
  - the excluded volume effect — no two monomers can occupy the same space;
  - attraction between monomers.
- In real polymers the balance between these two opposing effects is governed by temperature (equivalently, solvent efficiency).

Real chain phase transition

- In a good solvent or at high temperature the excluded volume effect dominates. Polymer chains are extended.
- In a poor solvent or at low temperature the attractive forces dominate and the polymer collapses into a localized phase.
- For a given solvent, there is a phase transition temperature (the θ-point) at which the two opposing effects essentially cancel.

Self-avoiding walk

- The traditional model for polymer chains in good solvent (where the excluded volume effect dominates) is self-avoiding walk (SAW) on $\mathbb{Z}^d$.



- SAW is conjectured to be super-diffusive for $d \in \{2, 3\}$, e.g., heuristic arguments (building on work of P.J. Flory from the 1940s) suggest $\|X_n\| \approx n^{3/4}$ in $d = 2$.
- But, SAW is not a progressive stochastic process
- **Challenge:** produce genuine stochastic processes that replicate some of the behaviour of (or conjectured for) SAW.

A new model

- We want a random walk model for polymer chains (X_n), $n = 1, 2, \ldots$, $X_n \in \mathbb{R}^d$.
- We want it to be a genuine stochastic process, in that conditional on $(X_1, \ldots, X_n)$, X_{n+1} has some (reasonably simple) distribution.
- Our choice of scale means $\|X_{n+1} - X_n\| = 1$.
- Our model needs to be flexible enough to model the full range of polymer phases:
  - collapsed (sub-diffusive motion);
  - θ-point (diffusive);
  - extended (super-diffusive, à la SAW).

Barycentric self-interaction

- To respect the motivation, our walk will have some self-interaction. We want a progressive process, so X_{n+1} interacts only with the past $X_1, \ldots, X_n$ (unlike SAW).
- Specifically, the self-interaction will be mediated by the centre of mass (barycentre) of the previous trajectory

$$G_n := \frac{1}{n} \sum_{i=1}^{n} X_i .$$

- Assume that there is some nice (Borel) kernel f such that

$$\mathbb{P}[X_{n+1} \in A \mid X_1, \ldots, X_n] = f(A; X_n, G_n), \text{ a.s.},$$

for all (Borel) $A \subseteq \mathbb{R}^d$.

Self-interaction

- Since $G_{n+1} = (nG_n + X_{n+1})/(n+1)$, this implies that (X_n, G_n) is a Markov process. Note that (X_n) itself is not Markovian in general.
- The key to our self-interaction will be an asymptotically zero drift of X_{n+1} towards or away from G_n. That is

$$\mathbb{E}[X_{n+1} - X_n \mid X_1, \ldots, X_n] = \rho \|X_n - G_n\|^{-\beta} \mathbf{u}(X_n - G_n),$$

where $\rho \in \mathbb{R}$ and $\beta > 0$ are fixed parameters and $\mathbf{u}(\mathbf{x}) := \mathbf{x}/\|\mathbf{x}\|$.

Example

- For $\mathbf{x} \in \mathbb{R}^d$, let $\mathbf{b}_1(\mathbf{x}), \ldots, \mathbf{b}_d(\mathbf{x})$ denote an orthonormal basis for $\mathbb{R}^d$ such that $\mathbf{b}_1(\mathbf{x}) = \mathbf{u}(\mathbf{x})$.
- For $i \in \{2, \ldots, d\}$, take

$$\mathbb{P}[X_{n+1} - X_n = \pm \mathbf{b}_i(X_n - G_n) \mid X_1, \ldots, X_n] = \frac{1}{2d}.$$

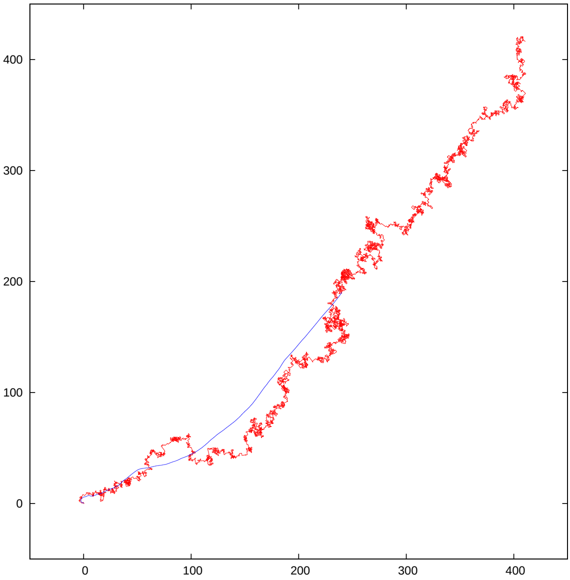
- Also (with a correction if $\|X_n - G_n\|$ is small) set

$$\mathbb{P}[X_{n+1} - X_n = \pm \mathbf{b}_1(X_n - G_n) \mid X_1, \ldots, X_n] = \frac{1}{2d} \pm \frac{\rho}{2} \|X_n - G_n\|^{-\beta}.$$

- Analogue of our centrally biased walk example with repulsion or attraction not from a fixed origin but from G_n.

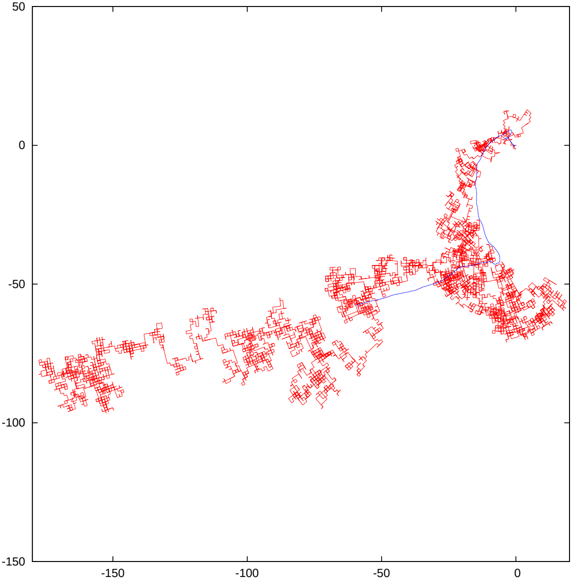
Example simulation 1

10^4 steps with $d = 2$, $\rho = 0.1$, $\beta = 0.1$.



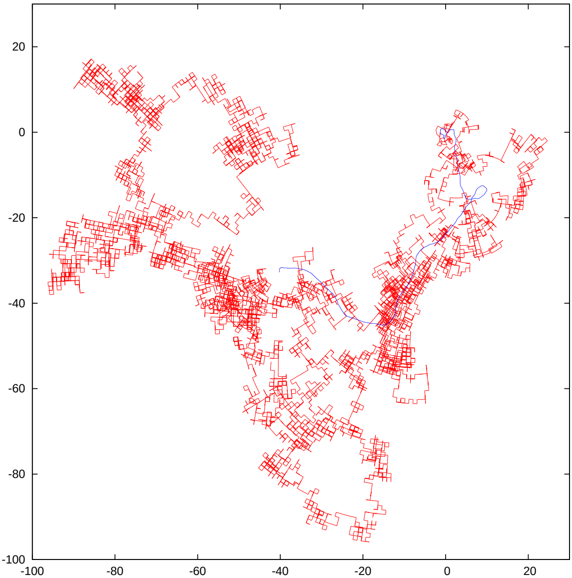
Example simulation 2

10^4 steps with $d = 2$, $\rho = 0.1$, $\beta = 0.5$.



Example simulation 3

10^4 steps with $d = 2$, $\rho = 0.1$, $\beta = 1$.



Questions

- For which values of the parameters (d, β, ρ) is X_n recurrent? Or transient?
- If X_n is transient, how rapidly does it escape to infinity? Is there a limiting direction?
- What information can we get about the process G_n? Or joint information about (X_n, G_n)?

Lyapunov function

- We try to find a suitable transformation of our self-interacting walk X_n into a tractable one-dimensional problem.
- The function we consider should presumably involve both X_n and G_n. A natural choice is $Z_n = \|X_n - G_n\|$. Then Z_n is a one-dimensional non-Markov process, but we might hope it satisfies Lamperti-type conditions.
- In fact, we get

$$\mathbb{E}[Z_{n+1} - Z_n \mid X_1, \ldots, X_n] \approx \rho' Z_n^{-\beta} - \frac{Z_n}{n}.$$

  There is an extra term in the drift; it is now time inhomogeneous.
- Also

$$\mathbb{E}[(Z_{n+1} - Z_n)^2 \mid X_1, \ldots, X_n] \approx \frac{1}{d}.$$

Lyapunov function (cont.)

- As a first guess, we can solve the corresponding differential equation:

$$\frac{\mathrm{d}z}{\mathrm{d}n} = \rho' z^{-\beta} - \frac{z}{n},$$

  to get $z = \mathrm{const.} n^{1/(1+\beta)}$. So we expect the terms $Z_n^{-\beta}$ and Z_n/n to be of the same size.
- Thus the starting point of our analysis of the self-interacting walk X_n is the study of this time-inhomogeneous analogue of Lamperti's problem for processes with drifts of the given form.

Recurrence classification for $X_n - G_n$

Let $\rho_0 := \frac{2-d}{2d}$.

Theorem (CMVW 2011)

Suppose that $d \in \mathbb{N}$. Let $Y_n := X_n - G_n$.

(i) *If $\beta > 1$, Y_n is recurrent if $d \in \{1, 2\}$ and transient if $d \geq 3$.*

(ii) *If $\beta = 1$, Y_n is recurrent if $\rho \leq \rho_0$ and transient if $\rho > \rho_0$.*

(iii) *If $\beta \in (0, 1)$, Y_n is recurrent if $\rho < 0$ and transient if $\rho > 0$.*

- So in particular if $\beta = 1$ and $d = 2$, $X_n - G_n$ is transient for any $\rho > 0$.
- How to convert this into a result about X_n? Some progress based on the useful formula $G_n = X_1 + \sum_{j=2}^{n} \frac{Y_j}{j-1}$.

Results for X_n: $\beta \in (0,1)$, $\rho > 0$

When $\beta \in (0,1)$, $\rho > 0$ we have a strong push away from the centre of mass. Here we get super-diffusive behaviour. By choice of β we can tune the model to (approximately) match SAW-scaling.

Theorem (CMVW 2011)

Suppose $\rho > 0$, $\beta \in (0,1)$. Then X_n is transient ($\|X_n\| \to \infty$ a.s.) with a limiting direction, i.e., $\mathbf{u}(X_n) \to \mathbf{u}$ a.s. for some (random) unit vector $\mathbf{u}$. Moreover there is a law of large numbers

$$n^{-\frac{1}{1+\beta}} \|X_n\| \to \lambda'(\rho, \beta) \quad \text{(constant) a.s.}$$

Results for X_n: $\beta = 1$

The case $\beta = 1$ is most delicate. Here we currently only have partial results, including:

- The complete recurrence classification for $X_n - G_n$ (see above) but not X_n itself (unless $d = 1 \ldots$).
- Bounds on $\|X_n\|$. Again depending on ρ, we can obtain diffusive bounds $\|X_n\| \approx n^{1/2}$, or, with some attraction (ρ negative) sub-diffusive bounds $\|X_n\| \approx n^{\nu}$ for $\nu < 1/2$.

We expect (but cannot yet prove) that there is no limiting direction in the $\beta = 1$ case, even when $X_n - G_n$ (or X_n) is transient.

Back to simple random walk

Now let X_n be SRW on $\mathbb{Z}^d$. How does $G_n = n^{-1} \sum_{i=1}^{n} X_i$ behave? What about the joint behaviour of (X_n, G_n)?

Theorem (Grill 1988)

For G_n the centre-of-mass process for SRW,

- *G_n is recurrent for $d = 1$;*
- *G_n is transient for $d \geq 2$.*

Centre of mass for SRW

For SRW, let $Z_n = \|X_n - G_n\|$. Now

$$\mathbb{E}[Z_{n+1} - Z_n \mid X_1, \ldots, X_n] \approx \frac{1}{2}\left(1 - \frac{1}{d}\right) Z_n^{-1} - \frac{Z_n}{n},$$

and

$$\mathbb{E}[(Z_{n+1} - Z_n)^2 \mid X_1, \ldots, X_n] \approx \frac{1}{d}.$$

This is exactly of the form that arose in our calculations for the self-interacting random walk. It follows from our results that:

Theorem (CMVW 2011)

For SRW,

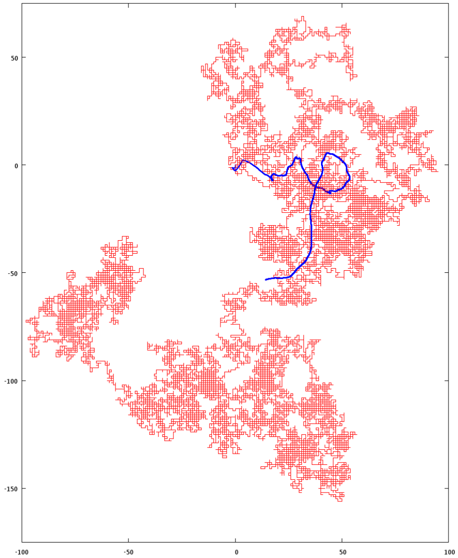
- $X_n - G_n$ *is recurrent for* $d \in \{1, 2\}$*;*
- $X_n - G_n$ *is transient for* $d \geq 3$*.*

Two dimensions

- **Amusing fact:** Setting $\Delta_n := X_{n+1} - X_n$, we have $G_n = \sum_{i=0}^{n-1}(1 - \frac{i}{n})\Delta_i$, while $X_n - G_n = \sum_{i=1}^{n}(1 - \frac{i}{n})\Delta_i'$ where $\Delta_i' = \Delta_{n-i}$. So for fixed n, G_n and $X_n - G_n$ are very nearly time reversals of each other, and so have basically the same (marginal) distributions. But as processes they are very different, e.g., in $d = 2$, G_n is transient (Grill) but $X_n - G_n$ is recurrent.
- So in $d = 2$ we have that X_n is recurrent while G_n heads off to infinity, but infinitely often X_n and G_n approach within distance 1 (say) of each other.

Picture

Picture: 4×10^4 steps of SRW and its centre of mass.



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