Partial Differential Equations and Random Walks

with Emphasis on the Heat Equation

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Agenda

Setting the Stage I

A Random Walk is a mathematical formalization of a path that contains random steps. This presentation will *briefly* show how the Heat Equation, a basic model that describes heat diffusing randomly in all directions at a specific rate, can be applied to study Random Walks. We will specifically explore Random Walk and the Discrete Heat Equation.

1D Random Walk I

Lets start by looking at Random Walks on integers:

- At each time unit, a walker can walk either up or down
- Framework: $P_{up}(X_j = 1) = 0.5, \quad P_{down}(X_j = -1) = 0.5$, S_n is position at step n

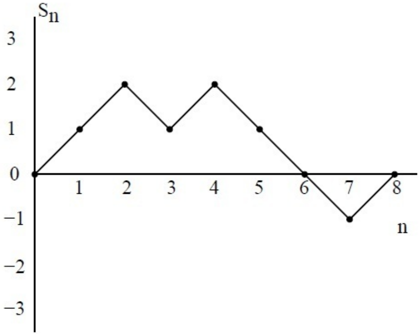

Figure: 1D Random Walk starting at $x = 0$

1D Random Walk II

Some facts and results:

- expectation and variance (starting at $x = 0$):

$$E[S_n] = 0 \quad Var[S_n] = n \tag{1}$$

- recall Stirling's Formula:

$$n! = \sqrt{2\pi} n^{n+\frac{1}{2}} e^{-n} [1 + O(\frac{1}{n})] \tag{2}$$

- Using Binomial Distribution, Central Limit Theorem, and (2) we get:

$$\lim_{x\to\infty} P(a\sqrt{2n} \leq S_{2n} \leq b\sqrt{2n}) = \frac{1}{\sqrt{2\pi}} \int_a^b \mathrm{e}^{-x^2/2}\, \mathrm{d}x \tag{3}$$

Theorem 1.1

The probability that a 1D simple random walker returns to the origin infinitely often is one (n must be even).

1D Boundary Value Problems

Consider the 1D Gambler's Ruin Problem: Suppose N is a positive integer and a random walker starts at $x \in \{0, 1, \ldots\ldots N\}$. Let S_n denote the position of the walker at time n. Suppose the walker stops when he reaches 0 or N.

- Define $T = \min\{n : S_n = 0\, or\, N\}$
- Define $F(x) = P(S_T = N | S_0 = x)$ note that $F(0) = 0$, $F(N) = 1$ and $F(x) = \frac{1}{2}F(x+1) + \frac{1}{2}F(x-1)$
- The position of walker at time n is given by $S_{n \wedge T}$, where $n \wedge T$ is the minimum of n and T.

Theorem 2.1

The only function $F : \{0, \ldots, N\} \to \mathbb{R}$ *that satisfies the above properties is*

$$F(x) = E(F(S_{n \wedge T})) = x/N \tag{4}$$

Random Walk on Several Dimensions I

We now consider a random walker on d-dimensional integer grid:

- $\mathbb{Z}^d = \{(x_1, \ldots x_d) : x_j \text{ are integers}\}$
- So now each step, the walker chooses one of its $2d$ nearest lattices, each with probability $1/2d$, to move to the lattice.
- Like before $S_n = x + X_1 + \ldots + X_d$, where $x, X_1, \ldots, X_d$ are unit vectors in that specific component.

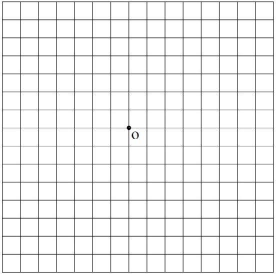

Figure: Random Walk on $\mathbb{Z}^2$ starting at $x = 0$

Random Walk on Several Dimensions II

Like the 1D case expectation and variance (starting at x):

$$E[S_n] = 0$$

$$Var[S_n] = n$$

Note here that $X_j \cdot X_j = 1$ and that:

$$X_j \cdot X_k = \begin{cases} 1 & \text{with probability } 1/2d \qquad j \neq k \\ -1 & \text{with probability } 1/2d \qquad j \neq k \end{cases}$$

Theorem 3.1

Suppose S_n, for n even, is a random walk on $\mathbb{Z}^d$ starting at the origin. If $d = 1, 2$ the random walk is recurrent (with probability 1 it returns to the origin). If $d \geq 3$, the random walk is transient (with probability one that it returns to the origin only finitely often). Note, if n is odd, the probability of it returning to the origin is 0.

Random Walk on Several Dimensions III

Proof.

If V is the number of visits to the origin and p is the probability that the d-dimensional walk returns to the origin, then

$$E[V] = \sum_{n=0}^{\infty} P(S_{2n} = 0) = 1/(1-p)\ (V \sim geometric)$$

By some work we can get $P(S_{2n} = 0) \sim c_d/n^{d/2}$, where $c_d = \frac{d^{d/2}}{\pi^{d/2} 2^{d-1}}$ So,

$$E[V] = \begin{cases} \leq \infty & d \geq 3 \\ \infty & d = 2 \end{cases}$$

□

Higher Dimension Boundary Value Problems

Suppose we have a finite subset $A \subseteq \mathbb{Z}^d$.

- The boundary of A is defined by:

$$\partial A = \{z \in \mathbb{Z}^d \setminus A : dist(z, A) = 1\} \tag{5}$$

- Define the discrete Laplacian, $\mathcal{L}$, as:

$$\mathcal{L}F(x) = \frac{1}{2d} \sum_{y \in \mathbb{Z}^d, |x-y|=1} [F(y) - F(x)] \tag{6}$$

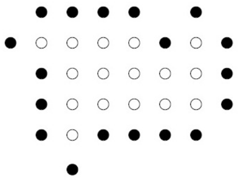

Figure: The white dots are A and the black dots are ∂A

Dirichlet Problem for Harmonic Functions I

Using S_n as te simple random walk on $\mathbb{Z}^d$. Then

$$\mathcal{L}F(x) = E[F(S_1) - F(S_0)|S_0 = x] \tag{7}$$

Dirichlet Problem for Harmonic Functions: Given a finite set A, $A \subseteq \mathbb{Z}^d$, and a function $F : \partial A \to \mathbb{R}$, find an extension of F to $\bar{A}$ such that

$$\mathcal{L}F(x) = 0 \ \ \forall x \in A \tag{8}$$

Theorem 4.1

If $A \subset \mathbb{Z}^d$ is finite and $T_A = \min\{n \geq 0 : S_n \notin A\}$, then for every $F : \partial A \to \mathbb{R}$, there is a (unique) extension of F to $\bar{A}$ that satisfies (8) and is given by

$$F_0(x) = E[F(S_{T_A})|S_0 = x] = \sum_{y \in \partial A} P(S_{T_A} = y|S_0 = x)F(y) \tag{9}$$

Dirichlet Problem for Harmonic Functions II

Proof.

This is the equivalent of solving a d-dimensional discrete Laplace equation. Using separation of variables, we will get the Poisson Kernel, $[H_A(x,y)]_{x \in A, y \in \partial A}$. Another way of stating this is to say that:

$$H_A(x,y) = P(S_{T_A} = y | S_0 = x) \tag{10}$$

So for a given set A, we can solve the Dirichlet problem for any boundary function in terms of the Poisson kernel. □

Dirichlet Problem for Harmonic Functions III

Example 1 (Deriving the Laplace Kernel)

Consider the Laplace Equation in two dimension on the boundary of a disk:

$$\mathcal{L}F(x,y) = f \tag{11}$$

Since we are solving this on a disk with radius,a,we transform it into polar coordinates. Then the solution of becomes:

$$F(r,\theta) = \frac{A_0}{2} + \sum_{1}^{\infty} A_n \frac{r^n}{a^n}\cos(n\theta) + B_n \frac{r^n}{a^n}\sin(n\theta) \tag{12}$$

where $A_n = \frac{1}{\pi}\int_{-\pi}^{\pi} f(\phi)\cos(n\phi)d\phi$ *and* $B_n = \frac{1}{\pi}\int_{-\pi}^{\pi} f(\phi)\sin(n\phi)d\phi$*.*

Note that because we are in the discrete case, we will just do Riemann sum instead whenever we see an integral.

Dirichlet Problem for Harmonic Functions IV

Example 2 (Deriving the Laplace Kernel Continued)

After some manipulation we can get:

$$F(r,\theta) = \int_{-\pi}^{\pi} f(\phi) P(r, \theta - \phi) d\phi \tag{13}$$

Where $P(r,\theta)$ is the Poisson Kernel

$$P(r,\theta) = \frac{1}{2\pi}[1 + 2\sum_{n=1}^{\infty} \frac{r^n}{a^n}\cos(n\theta)] = \frac{1}{2\pi}\frac{a^2 - r^2}{a^2 + r^2 - 2ar\cos(\theta)} \tag{14}$$

Properties of the Poisson Kernel:

- $\int_{-\pi}^{\pi} P(r,\theta) d\theta = 1$
- $P(r,\theta) > 0$ *for* $0 \leq r < a$
- $\forall \epsilon > 0 \lim_{r \to a^-} P(r,\theta) d\theta = 0$

Discrete Heat Equation Set-up I

Let A be a finite subset of $\mathcal{Z}^d$ with boundary ∂A. Set temperature at the boundary to be 0 at all times and set the temperature at $x \in A$ to be $p_n(x)$. At each integer time unit n, the heat at x at time n is spread evenly among its $2d$ neighbours. If one of the neighbours is a boundary point, then the heat that goes to that point is lost forever. So let,

$$p_{n+1}(x) = \frac{1}{2d} \sum_{|y-x|=1} p_n(y) \tag{15}$$

Let $\partial_n p_n(x) = p_{n+1} - p_n$ and we get the *heat equation*:

$$\partial_n p_n(x) = \mathcal{L} p_n(x), \quad x \in A \tag{16}$$

The initial temperature is given as an initial condition

$$p_0(x) = f(x), \quad x \in A \tag{17}$$

Discrete Heat Equation Set-up II

The boundary condition is given as

$$p_n(x) = 0, \quad x \in \partial A \tag{18}$$

If $x \in A$ and the initial condition is $f(x) = 1$ and $f(z) = 0$ for $z \neq x$, then

$$p_n(y) = P(S_{n \wedge T_A} = y | S_0 = x) \tag{19}$$

Given any initial condition f, there is a unique function p_n that satisfies (16)-(18)and that the set of functions satisfying (16)-(18) is a vector space with the same dimension as A. In fact, $\{p_n(x) : x \in A\}$ is the vector $\mathcal{Q}^n f$. Such that:

$$\mathcal{Q}F(x) = \frac{1}{2d} \sum_{y \in \mathbb{Z}^d, |x-y|=1} F(y), \quad \mathcal{L}F(x) = (\mathcal{Q} - \mathcal{I})F(x) \tag{20}$$

Discrete 1-D Heat Equation I

In trying to solve p_n for $A = 1, \ldots, N-1$, we start by looking for functions satisfying (16) of the form

$$p_n(x) = \lambda^n \phi(x) \tag{21}$$

$$\partial_n p_n(x) = \lambda^{n+1}\phi(x) - \lambda^n \phi(x) = (\lambda - 1)\lambda^n \phi(x) \tag{22}$$

This nice form leads us to try to eigenvalue and eigenfunctions of $\mathcal{Q}$, i.e to find λ, ϕ such that

$$\mathcal{Q}\phi(x) = \lambda\phi(x), \quad \text{with} \quad \phi \equiv 0 \quad \text{on} \quad \partial A \tag{23}$$

Instead of using characteristic polynomials, we will make good guesses.

Discrete 1-D Heat Equation II

From $\sin((x \pm 1)\theta) = \sin(x\theta)\cos(\theta) \pm \cos(x\theta)\sin(\theta)$, we can get

$$\mathcal{Q}\{\sin(\theta x)\} = \lambda_\theta\{\sin(\theta x)\},\ \lambda_\theta = \cos(\theta) \tag{24}$$

Choosing $\theta_j = \pi j/N$, then $\phi_j(x) = \sin(\pi jx/N)$ and satisfies the boundary condition $\phi_j(0) = \phi_j(N) = 0$. Since these are eigenvectors with different eigenvalues for a symmetric matrix, then they must be orthogonal and linearly independent.So then every function f on A can be written in a unique way:

$$f(x) = \sum_{j=1}^{N-1} c_j \sin(\frac{\pi jx}{N}) \tag{25}$$

Then the solution with heat equation with initial condition f is

$$p_n(y) = \sum_{j=1}^{N-1} c_j[\cos(\frac{j\pi}{N})]^n \phi_j(y) \tag{26}$$

Discrete 1-D Heat Equation III

In particular, if we choose the solution with initial condition $f(x) = 1$ and $f(z) = 0$ for $z \neq x$, then

$$p_n(y) = P(S_{n \wedge T_A} = y | S_0 = x) = \frac{2}{N} \sum_{j=1}^{N-1} \phi_j(x) [\cos(\frac{j\pi}{N})]^n \phi_j(y) \qquad (27)$$

note that we used the double-angle formula and $\sum_{j=1}^{N} \cos(\frac{2k\pi}{N}) = \sum_{j=1}^{N} \sin(\frac{2k\pi}{N}) = 0$ to get:

$$\sum_{j=1}^{N-1} \sin^2(\frac{\pi j x}{N}) = \frac{N}{2} \qquad (28)$$

Discrete 1-D Heat Equation IV

As $n \to \infty$, the sum becomes very small but it is dominated by $j = 1$ and $j = N - 1$ terms, which the eigenvalue has the maximal absolute value. These 2 terms give:

$$\frac{2}{N}\cos^n(\frac{\pi}{N})[\sin(\frac{\pi x}{N})\sin(\frac{\pi y}{N}) + (-1)^n \sin(\frac{\pi(N-1)x}{N})\sin(\frac{\pi(N-1)y}{N}] \tag{29}$$

and hence if $x, y \in \{1, \ldots, N-1\}$, as $n \to \infty$,

$$P(S_{n \wedge T_A} = y | S_0 = x) \sim \frac{2}{N}\cos^n(\frac{\pi}{N})[1 + (-1)^{n+x+y}]\sin(\frac{\pi x}{N})\sin(\frac{\pi y}{N}) \tag{30}$$

Discrete 1-D Heat Equation V

So for large n, such that the walker has not left $\{1, \ldots, N-1\}$, the probability that the walker is at y is about $c\sin(\frac{\pi y}{N})$ assuming that $n + x + y$ is even. Other than this assumption, there is no dependence on the starting point x for the limiting distribution. Also, it is important to notice that the walker is more likely to be at the points toward the middle of the interval.

Discrete Multidimensional Heat Equation I

Extending the theory of 1-D Heat Equation, we get the following

Theorem 5.1

If A is a finite subset of $\mathbb{Z}^d$ with N elements, then we can find N linearly independent functions $\phi_1, \ldots, \phi_N$ that satisfy (24) with real eigenvalues $\lambda_1, \ldots, \lambda N$. The solution to (16)-(18)is given by:

$$p_n(x) = \sum_{j=1}^{N} c_j \lambda_j^n \phi_j(x) \tag{31}$$

Where c_j are chosen so that

$$f(x) = \sum_{j=1}^{N} c_j \phi_j(x) \tag{32}$$

The ϕ_j can be chosen to be orthonormal.

Discrete Multidimensional Heat Equation II

Since $p_n(x) \to 0$ as $n \to \infty$, we can order the eigenvalues such that:

$$1 > \lambda_1 \geq \lambda_2 \geq \ldots \geq \lambda_N > -1 \tag{33}$$

Let $p(x, y; A) = P(S_{n \wedge T_A} = y | S_0 = x)$. Then if the dimension of $A = N$:

$$p(x, y; A) = \sum_{j=1}^{N} c_j(x) \lambda_j^n \phi_j(y) \tag{34}$$

Where $c_j(x)$ was chosen so that it is orthonormal to $\phi_j(y)$. So then this implies that $c_j(x) = \phi_j(x)$. Hence:

$$p(x, y; A) = \sum_{j=1}^{N} \phi_j(x) \phi_j(y) \lambda_j^n \tag{35}$$

Discrete Multidimensional Heat Equation III

Let the largest eigenvalue, λ_1, be denoted as λ_A. Then we can give a definition of λ_A using the theorem about the largest eigenvalue of symmetric matrices:

Theorem 5.2

If A is a finite subset of $\mathbb{Z}^d$, then λ_A is given by:

$$\lambda_A = \sup_f \frac{\langle \mathcal{Q}f, f \rangle}{\langle f, f \rangle} \tag{36}$$

Where the supremum is over all functions f on A, and $\langle ., . \rangle$ denotes inner product:

$$\langle f, g \rangle = \sum_{x \in A} f(x) g(x) \tag{37}$$

Discrete Multidimensional Heat Equation IV

Using this formulation, we can see that the eigenfunction for λ_1 can be uniquely chosen so that $\phi_1(x) \geq 0$. If $x = (x_1, \ldots, x_d) \in \mathbb{Z}^d$, let $\text{par}(x) = (-1)^{x_1 + \ldots + x_d}$. We call x even if $\text{par}(x) = 1$ and otherwise x is odd. So if n is nonnegative integer then

$$p_n(x, y; A) = 0 \quad if \ (-1)^n \, \text{par}(x + y) = -1 \tag{38}$$

$$\mathcal{Q}[\text{par}(\phi)] = -\lambda \, \text{par}(\phi) \tag{39}$$

Theorem 5.3

Suppose A is a finite connect subset of $\mathbb{Z}^d$ with at least two points. Then $\lambda_1 > \lambda_2, \lambda_N = -\lambda_1 < \lambda_{N-1}$. The eigenfunction ϕ_1 can be chosen so that $\phi_1 > 0 \, \forall x \in A$.

$$\lim_{n \to \infty} \lambda_1^{-n} p_n(x, y; A) = [1 + (-1)^n \, \text{par}(x + y)] \phi_1(x) \phi_1(y) \tag{40}$$

Discrete Multidimensional Heat Equation V

Example 3

We can compute the eigenfunciton and eigenvalues exactly for a d-dimensional rectangle:

$$A = \{(x_1, \ldots, x_d) \in \mathbb{Z}^d : 1 \leq x_j \leq N_j - 1\} \tag{41}$$

Using the index $\bar{k} = (k_1, \ldots, k_d) \in A$, *we get the eigenfunctions and eigenvalue as:*

$$\phi_{\bar{k}}(x_1, \ldots, x_d) = \sin(\frac{k_1 \pi x_1}{N_1}) \sin(\frac{k_2 \pi x_2}{N_2}) \ldots \sin(\frac{k_d \pi x_d}{N_d}) \tag{42}$$

$$\lambda_{\bar{k}} = \frac{1}{d}[\cos(\frac{k_1 \pi}{N_1}) + \ldots + \cos(\frac{k_d \pi}{N_d})] \tag{43}$$

Possible Further Topics

Brownian and the Continuous Heat Equation

- Brownian Motion
- Harmonic Functions
- Dirichlet Problem
- Heat Equation
- Bounded Domain

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