THE HEAT EQUATION AND HARMONIC FUNCTIONS OVER GRAPHS

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Abstract. The following paper will first introduce the concept of a random walk and how it relates to the heat equation. The paper will look at simple random walks and the heat equation on different types of graphs, such as bipartite graphs and the integer lattice. We will also find harmonic functions on these graphs.

Contents

1. A Couple of Definitions

Before delving into random walks and the heat equation, we must first introduce some definitions in graph theory and probability. We begin with some definitions in graph theory.

Definition 1.1. A *simple graph* G consists of a *vertex set V(G)* and an *edge set E(G)*, whose elements are ordered pairs of distinct vertices.

Definition 1.2. An *undirected graph* is a simple graph G where for all $v_1, v_2 \in V(G)$, if $(v_1, v_2) \in E(G)$, then $(v_2, v_1) \in E(G)$.

Definition 1.3. The *degree* of a vertex v is the number of edges (v, u) that are in $E(G)$. The degree of a vertex v is denoted by $\deg(v)$.

Definition 1.4. Two vertices v_1 and v_2 are *adjacent* if $(v_1, v_2) \in E(G)$. If v_1 and v_2 are adjacent, we denote this by $v_1 \sim v_2$. As a side note, except in undirected graphs, adjacency is not an equivalence relation.

Definition 1.5. *Regular graphs* are graphs such that all vertices have the same degree.

Definition 1.6. A *path* in G is a list of vertices $(v_1, v_2, ...v_n)$ such that $v_i \sim v_{i+1}$.

Definition 1.7. A *connected graph* is a graph where for all $v_1, v_2 \in G$, there exists a path from v_1 to v_2.

We will also introduce a few definitions in probability.

Definition 1.8. An *event* is an element of a set of outcomes to which a probability is assigned.

Definition 1.9. A *discrete random variable* is a variable with values in a countable subset S of $\mathbb{R}$ and has a probability of taking on any value s in S. Furthermore, $\sum_{s\in S} \mathbb{P}(X = s) = 1$, $\mathbb{P}(X = s) \geq 0$, and $\mathbb{P}(X \in U) = \sum_{s\in U\cap S} \mathbb{P}(X = s)$.

Definition 1.10. The *expectation*, denoted as $\mathbb{E}$, is defined for a discrete random variable X as

$$\mathbb{E}(X) = \sum_z z\mathbb{P}(X = z).$$

Definition 1.11. Take Y_1 and Y_2 to be two events. The *conditional probability* of Y_1 given Y_2, denoted as $\mathbb{P}(Y_1|Y_2)$ is defined as

$$\mathbb{P}(Y_1|Y_2) = \frac{\mathbb{P}(Y_1 \cap Y_2)}{\mathbb{P}(Y_2)},$$

assuming $\mathbb{P}(Y_2) \neq 0$.

Definition 1.12. Take X to be a discrete random variable and Y to be an event. The *conditional expectation* of X given Y, denoted as $\mathbb{E}[X|Y]$ is defined as

$$\mathbb{E}[X|Y] = \sum_z (z \cdot \mathbb{P}(X = z|Y)) = \sum_z \left(z \cdot \frac{\mathbb{P}((X = z) \cap Y)}{\mathbb{P}(Y)}\right)$$

assuming $\mathbb{P}(Y) \neq 0$.

2. Random Walks

A random walk on a graph G is a process in which a "walker" starts at a certain vertex, and at every time interval, the walker moves to an adjacent vertex. In this paper, we will look at simple random walks on different kinds of graphs. A simple random walk is simply a random walk in which the walker has an equal chance of moving to any adjacent point. So, if at a certain time the random walker is located at a point adjacent to n other vertices, at the next time step, the walker has a $1/n$ chance to move to each adjacent vertex. The simple random walk is time-independent — the time the walker reaches a certain point does not affect the transition probabilities from that point.

The transfer of heat can be modeled using random walks. Consider a graph G. Heat can be modeled by imagining a large number of particles starting at a position on the graph, and these particles performing random walks throughout the graph. At any time, the temperature at a point is the density of the particles at that point.

Let $p_n(x)$ denote the temperature (or the density of particles) at point x in G at time n. Between time n and time $n + 1$, heat flows into point x from all adjacent points in G. Then, the expected heat at time $n + 1$ at point x is

$$p_{n+1}(x) = \sum_{y\sim x,\ y\in G} p_n(y) \frac{1}{\deg(y)}.$$

3. Harmonic Functions

We will define two operators Q and L on functions $F : V(G) \to \mathbb{R}$ as follows:

$$QF(x) = \frac{1}{\deg(x)} \sum_{y \sim x,\ y \in G} F(y)$$

$$LF(x) = (Q - I)F(x) = \frac{1}{\deg(x)} \sum_{y \sim x,\ y \in G} F(y) - F(x)$$

The linear operator L is called the discrete Laplacian. With regards to the heat equation on the integer lattice (or other regular graphs), if $F(x)$ is the temperature at x at a time step n for all $x \in G$, then $QF(x)$ is the function describing the temperature on the graph at time step $n + 1$. Also, $LF(x)$ gives the change in temperature at point x from time n to time $n + 1$.

Definition 3.1. A function F is *harmonic* on x if $LF(x) = 0$. Furthermore, a function F is *harmonic* on A if $LF(x) = 0$ for all $x \in A$.

For the heat equation, if F is harmonic on a regular graph, then F is at an equilibrium — the temperature at each point on the graph remains the same. In this paper we will consider harmonic functions on different types of graphs.

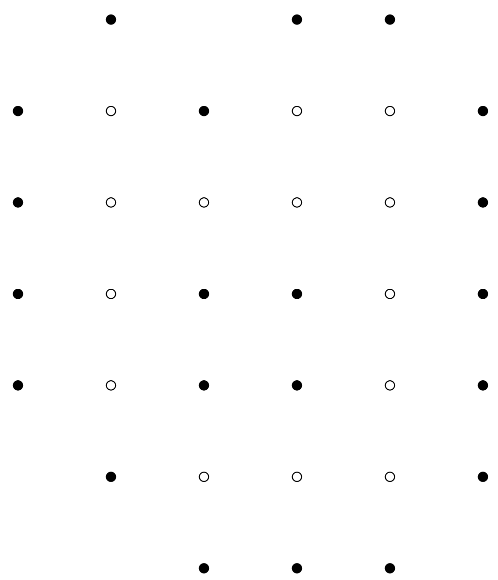
4. Boundary Value Problems

We will consider finite connected graphs with boundary values. We will define the boundary of a graph as follows. Given any finite connected graph G, we can choose a set of points ∂A such that the rest of the points are connected. Then, we call ∂A a boundary of the graph and denote the rest of the graph $(G - \partial A)$ as A. Also, we will let T_A be the first time a random walker reaches a boundary point. S_n will denote the location of the random walker at time n.

First, let us consider finite connected subsets of $\mathbb{Z}^d$. In the case of a subset, A, of $\mathbb{Z}^d$, ∂A can be defined as

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

The following is an example on $\mathbb{Z}^2$, where the white dots are on A and the black dots represent the boundary ∂A.



Theorem 4.1. *If A is a finite, connected subset of $\mathbb{Z}^d$, for a function $F : \partial A \to \mathbb{R}$, there exists a unique extension of F to $A \cup \partial A$ such that F is harmonic for all x in A. The extension of F is as follows:*

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

Before proving this theorem, we will define a martingale.

Definition 4.2. For a random walk, a process that satisfies $\mathbb{E}[M_{n+1}|S_0, \dots, S_n] = M_n$ is called a *martingale*.

Proof. Let F be a harmonic function on A. Let $n \wedge T_A$ denote the minimum of n and T_A. Then, let $M_n = F(S_{n \wedge T_A})$.

First, let's consider the case where $n < T_A$. Then, the expected value of M_{n+1} given the location of the walker at time n (let's call this x) is $\frac{1}{\deg(x)} \sum_{y \sim x} F(y)$. Because $LF(x) = 0$, this equals $F(x) = F(S_{n \wedge T_A})$. So,

$$\mathbb{E}[M_{n+1}|S_0, \dots, S_n] = F(S_{n \wedge T_A}) = M_n.$$

Let's say that the random walker starts at point x ($S_0 = x$). We will show that $\mathbb{E}[M_{n+1}] = \mathbb{E}[M_n]$.

$$\begin{aligned} \mathbb{E}[M_{n+1}] &= \mathbb{E}[F(S_{(n+1) \wedge T_A})] \\ &= \sum_{y \in A \bigcup \partial A} \mathbb{P}\left(S_{n \wedge T_A} = y | S_0 = x\right) \mathbb{E}[F(S_{(n+1) \wedge T_A}) | S_{n \wedge T_A} = y] \\ &= \sum_{y \in A \bigcup \partial A} \mathbb{P}\left(S_{n \wedge T_A} = y | S_0 = x\right) \left(\sum_{x \sim y} \frac{1}{\deg(y)} F(x) \right) \end{aligned}$$

Note that because $LF(x) = 0$, $\sum_{x\sim y} \frac{1}{\deg(y)} F(x) = F(y)$,

$$\mathbb{E}[M_{n+1}] = \sum_{y\in A\bigcup \partial A} \mathbb{P}(S_{n\wedge T_A} = y|S_0 = x)F(y) = \mathbb{E}[M_n].$$

So, via induction, $\mathbb{E}[M_{n+1}] = \mathbb{E}[M_n] = \ldots = \mathbb{E}[M_0]$. This proof can be generalized to any martingale to show that $\mathbb{E}[M_n] = \mathbb{E}[M_0]$. However, since this result is not necessary for the rest of the paper, it won't be proven here.

If we let n be equal to $T_A - 1$, we note that then $\mathbb{E}[M_{T_A}] = \mathbb{E}[M_0]$. For cases where $n \geq T_A$, $\mathbb{E}[S_n] = \mathbb{E}[S_{T_A}] = \mathbb{E}[M_0]$.

Then,

$$\sum_{y\in A\cup\partial A} \mathbb{P}(S_{n\wedge T_A} = y|S_0 = x)F(y) = \mathbb{E}[M_n] = \mathbb{E}[M_0] = F(x). \tag{4.3}$$

For a finite graph, the random walker will, with probability one, reach a boundary point in a finite amount of time. Thus, if we take $\lim_{n\to\infty}$ of equation (4.3), we get that

$$F(x) = \sum_{y\in\partial A} \mathbb{P}(S_{T_A} = y|S_0 = x)F(y). \tag{4.4}$$

To show that this is a unique solution, suppose that F_1 and F_2 are two harmonic functions on a graph with boundary conditions. Then, since the difference between two harmonic functions is also harmonic (since both Q and L are linear in F), $(F_1 - F_2)$ is also harmonic. Note that then the boundary conditions all have a value of 0. Because $LF(x)$ is the difference between $F(x)$ and the average of the values of the neighbors of x, if $F(x) = 0$ for all $x \in \partial A$, for $F(x)$ to be harmonic on the graph, the function must equal 0 on all points on A. Thus, $F_1(x) = F_2(x)$. □

Note that Theorem 4.1 applies not only to finite subsets of $\mathbb{Z}^d$ but also to any regular graph in which a random walker almost surely reaches a boundary point in a finite number of steps.

So, given a function $F : \partial A \to \mathbb{R}$, we can find a unique function $F_0 : A\cup\partial A \to \mathbb{R}$ such that $LF_0(x) = 0$ for all x in A. If ∂A has m elements and A has n elements, finding the harmonic function on $A \cup \partial A$ is a transformation from a vector in $\mathbb{R}^m$ to a vector in $\mathbb{R}^{m+n}$. It is the identity over the first m elements. F is a linear transformation from $\mathbb{R}^m$ to $\mathbb{R}^n$.

To show that this is a linear transformation: Take two functions on the boundaries $F : \partial A \to \mathbb{R}$ and $G : \partial A \to \mathbb{R}$. Then,

$$\begin{aligned}(F + G)_0(x) &= \sum_{y\in\partial A} \mathbb{P}(S_{T_A} = y|S_0 = x)(F + G)(y) \\ &= \sum_{y\in\partial A} \mathbb{P}(S_{T_A} = y|S_0 = x)F(y) + \sum_{y\in\partial A} \mathbb{P}(S_{T_A} = y|S_0 = x)G(y) \\ &= F_0(x) + G_0(x).\end{aligned}$$

Also, if we multiply the function F by λ to get a function $\bar{F}$,

$$(\bar{F})_0(x) = \sum_{y\in\partial A} \mathbb{P}(S_{T_A} = y|S_0 = x)\bar{F}(y) = \lambda \sum_{y\in\partial A} \mathbb{P}(S_{T_A} = y|S_0 = x)F(y) = \lambda F_0(x).$$

We can write the linear transformation as a matrix $\mathbf{H}_A$, which we will call the Poisson kernel.

Definition 4.5. We define the *Poisson kernel* $\mathbf{H}_A$ for a graph A with boundary ∂A as the $n \times m$ matrix where

$$\mathbf{H}_A = [H_A(x,y)]_{x\in A, y\in\partial A}$$
$$\text{where } H_A(x,y) = \mathbb{P}\left(S_{T_A} = y | S_0 = x\right)$$

Then, given a function $F : \partial A \to \mathbb{R}$, the harmonic function on A is

$$F_0(x) = \sum_{y\in\partial A} H_A(x,y)F(y). \tag{4.6}$$

Or, equivalently, if F and F_0 are written as column matrices, $F_0 = \mathbf{H}_A \cdot F$.

5. Examples Over the Integer Lattice

Example 1. Now we consider a finite subset of $\mathbb{Z}$ with boundary conditions at the ends. We take A to be $\{1,\ldots,N-1\}$ and ∂A to be $\{0,N\}$. Let $F(0) = a$ and $F(N) = b$.

Theorem 5.1. *Given the above conditions, the only function F that is harmonic on A is*

$$F(x) = a + \frac{x(b-a)}{N} \tag{5.2}$$

Proof. It is easy to see that F is harmonic. In this case, $LF(x) = 0$ is equivalent to saying

$$\frac{1}{2}[F(x+1) - F(x-1)] = F(x),$$

which is true for $F(x) = a + \frac{x(b-a)}{N}$. By Theorem 4.1, this is the unique solution. □

Example 2. Now, as another, less trivial example, consider the following square in $\mathbb{Z}^2$. Let

$$A = \{(x_1,x_2) : x_j = 1,\ldots,N-1\}$$

Then, the boundary of A can be split up into four portions, which can be written as

$$\begin{aligned}
\partial A &= \partial_{1,0} \cup \partial_{1,N} \cup \partial_{2,0} \cup \partial_{2,N} \\
\partial_{1,0} &= \{(0,x_2) : x_2 = 1,\ldots,N-1\} \\
\partial_{1,N} &= \{(N,x_2) : x_2 = 1,\ldots,N-1\} \\
\partial_{2,0} &= \{(x_1,0) : x_1 = 1,\ldots,N-1\} \\
\partial_{2,N} &= \{(x_1,N) : x_1 = 1,\ldots,N-1\}.
\end{aligned}$$

Let h_j be the function

$$h_j(x) = \sinh\left(\frac{\beta_j x_1}{N}\right)\sin\left(\frac{j\pi x_2}{N}\right). \tag{5.3}$$

β_j is a constant that will be defined later. Now, consider what $Lh_j(x)$ is equal to. We will use the angle sum formulas for sin and sinh, which are as follows:

$$\sin(a+b) = \sin(a)\cos(b) + \cos(a)\sin(b)$$
$$\sinh(a+b) = \sinh(a)\cosh(b) + \cosh(a)\sinh(b)$$

Using the angle sum formulas, we can calculate what $Lh_j(x)$ is equal to.

$$\begin{aligned}
Lh_j(x) = \ & \frac{1}{4}\Bigg[\sinh\left(\frac{\beta_j(x_1+1)}{N}\right)\sin\left(\frac{j\pi x_2}{N}\right)+\sinh\left(\frac{\beta_j(x_1-1)}{N}\right)\sin\left(\frac{j\pi x_2}{N}\right)\\
&+\sinh\left(\frac{\beta_j(x_1)}{N}\right)\sin\left(\frac{j\pi(x_2+1)}{N}\right)+\sinh\left(\frac{\beta_j(x_1)}{N}\right)\sin\left(\frac{j\pi(x_2-1)}{N}\right)\\
&-4\sinh\left(\frac{\beta_j x_1}{N}\right)\sin\left(\frac{j\pi x_2}{N}\right)\Bigg]\\
= \ & \frac{1}{4}\Bigg\{\sin\left(\frac{j\pi x_2}{N}\right)\Bigg[\sinh\left(\frac{\beta_j x_1}{N}\right)\cosh\left(\frac{\beta_j}{N}\right)+\cosh\left(\frac{\beta_j x_1}{N}\right)\sin\left(\frac{\beta_j}{N}\right)\\
&+\sinh\left(\frac{\beta_j x_1}{N}\right)\cosh\left(\frac{-\beta_j}{N}\right)+\cosh\left(\frac{\beta_j x_1}{N}\right)\sinh\left(\frac{-\beta_j}{N}\right)\Bigg]\\
&+\left(\sinh\left(\frac{\beta_j x_1}{N}\right)\right)\left(2\sin\left(\frac{x_2 j\pi}{N}\right)\cos\frac{j\pi}{N}\right)-4\sinh\left(\frac{\beta_j x_1}{N}\right)\sin\left(\frac{j\pi x_2}{N}\right)\Bigg\}
\end{aligned}$$

Because sinh is an odd function and cosh is an even function, this simplifies to

$$Lh_j(x)=\frac{1}{4}\left[2\sin\left(\frac{j\pi x_2}{N}\right)\sinh\left(\frac{\beta_j x_1}{N}\right)\left(\cosh\left(\frac{\beta_j}{N}\right)+\cos\left(\frac{j\pi}{N}\right)-2\right)\right].$$

If we choose β_j such that $\cosh\left(\frac{\beta_j}{N}\right)+\cos\left(\frac{j\pi}{N}\right)=2$, then $h_j(x)$ is harmonic on A. Note that such a β_j exists because $\cos\left(\frac{j\pi}{N}\right)$ ranges from -1 to 1 and changing β_j makes $\cosh\left(\frac{\beta_j}{N}\right)$ take on all values from 1 to infinity.

Note that on $\partial_{1,0}$, $\partial_{2,0}$, and $\partial_{2,N}$, $h_j(x)=0$. On $\partial_{1,N}$, $h_j(x)=\sinh(\beta_j)\sin\left(\frac{j\pi x_2}{N}\right)$. We will allow the values of $F(x)$ for $x\in\partial_{1,N}$ to vary and find the resulting harmonic functions on A.

This will require a few steps, which will be outlined here first. We will first look at just $\partial_{1,N}$. We will create a function f_y of k for a specific point (N,y) on the boundary such that $f_y(k)$ equals 1 if $k=y$ and equals 0 if $k\neq y$.

To do this, we will show that the $N-1$ functions $\sin(\frac{j\pi k}{N})$, for $j=1$ to $N-1$, form a basis for functions on $\partial_{1,N}$. As a result, there exist c_j's such that

$$f_y(k)=\sum_{j=1}^{N-1}c_j\sinh(\beta_j)\sin\left(\frac{j\pi k}{N}\right)=\begin{cases}1 & \text{if } k=y\\ 0 & \text{if } k\neq y.\end{cases}$$

Then, we show that

$$c_j=\frac{2}{N\sinh(b_j)}\sin(\frac{j\pi y}{N})$$

are the correct c_j's. Plugging in this value for c_j yields

$$f_y(k)=\sum_{j=1}^{N-1}\frac{2}{N}\sin(\frac{j\pi y}{N})\sin(\frac{j\pi k}{N}).$$

Then, we will show that if $k=y$, then $f_y(k)=1$, and if $k\neq y$, then $f_y(k)=0$.

So, for a specific point (N,y) on the boundary, we have a function $f_y(k)$ which equals 1 when $k=y$ and 0 if $k\neq y$. Then, if we are given any function on the boundary, we can simply take the sum of different $f_y(k)$'s. We then extend the function f_y to a function g_y of (x_1,x_2) such that $g_y(N,x_2)$ is equal to $f_y(x_2)$. So then, g_y is harmonic on A (because it is a sum of $\sinh(\frac{b_j x_1}{N})\sin(\frac{j\pi x_2}{N})$'s), is equal to

0 on $\partial_{1,0}$, $\partial_{2,0}$, and $\partial_{2,N}$, and is equal to f_y on $\partial_{1,N}$. Given a function F on $\partial_{1,N}$, the harmonic function on A is then

$$F(x_1, x_2) = \sum_{y \in (1,\dots,N-1)} F(N, y) g_y(x_1, x_2).$$

Now we begin the solution. We will first consider just $\partial_{1,N}$. The vector space of functions on $\partial_{1,N}$ is of dimension $N-1$. We will show that the functions $\{\sin\left(\frac{j\pi y}{N}\right)\}$ for $j = 1, \dots, N-1$ are linearly independent. First, we will show that the functions $\{\sin(\theta y)\}$ are eigenvectors of Q. To do this, we need to use the fact that

$$\sin(\theta(y \pm 1)) = \sin(y\theta)\cos(\theta) \pm \cos(y\theta)\sin(\theta).$$

With this, we can see that

$$\begin{aligned}
Q(\sin(\theta y)) &= \frac{1}{2}[\sin(\theta(y+1))) + \frac{1}{2}(\sin(\theta(y-1))] \\
&= \frac{1}{2}[\sin(y\theta)\cos(\theta) + \cos(y\theta)\sin(\theta) + \sin(y\theta)\cos(\theta) - \cos(y\theta)\sin(\theta)] \\
&= \sin(y\theta)\cos(\theta)
\end{aligned}$$

Then,

$$Q(\sin(\theta y)) = \lambda_\theta(\sin(\theta y)),\ \lambda_\theta = \cos\theta,$$

Now, we let $\theta = \frac{j\pi}{N}$. We see that $\{\sin(\frac{j\pi y}{N})\}$ for $j = 1, \dots, N-1$ is a group of $N-1$ eigenvectors with different eigenvalues. Also, note that Q is a symmetric matrix. As a result, these functions are pairwise orthogonal and thus linearly independent. Since $\partial_{1,N}$ contains $N-1$ elements, these $N-1$ functions form a basis for functions on $\partial_{1,N}$.

As a result, any function f on $\partial_{1,N}$ can be written as

$$f(y) = \sum_{j=1}^{N-1} c_j \sinh(\beta_j) \sin\left(\frac{j\pi y}{N}\right), \tag{5.4}$$

for some c_j's. Note that the $\sinh(\beta_j)$'s are constants.

For a fixed point $(1, y) \in \partial_{1,N}$, we can create a function that equals 1 at that point and 0 elsewhere. There exist c_j's such that

$$f_y(k) = \sum_{j=1}^{N-1} c_j \sinh(\beta_j) \sin\left(\frac{j\pi k}{N}\right) = \begin{cases} 1 & \text{if } k = y \\ 0 & \text{if } k \neq y. \end{cases} \tag{5.5}$$

Now, we will show that

$$c_j = \frac{2}{N\sinh(\beta_j)} \sin\left(\frac{j\pi y}{N}\right)$$

are the correct c_j's. Before we do, we need to show that $\sum_{j=1}^{N-1} \sin^2\left(\frac{j\pi y}{N}\right) = \frac{N}{2}$.

$$\begin{aligned}
\sum_{j=1}^{N-1} \sin^2\left(\frac{j\pi y}{N}\right) &= \sum_{j=1}^{N} \sin^2\left(\frac{j\pi y}{N}\right) && \text{because} \sin^2(j\pi) = 0 \\
&= \frac{1}{2}\sum_{j=1}^{N} [1 - \cos\left(\frac{2j\pi y}{N}\right)] && \text{because} \sin^2(x) = \frac{1-\cos(2x)}{2} \\
&= \frac{N}{2} - \frac{1}{2}\sum_{j=1}^{N} \cos\left(\frac{2j\pi y}{N}\right)
\end{aligned}$$

To see that $\sum_{j=1}^{N} \cos\left(\frac{2j\pi y}{N}\right) = 0$, consider the Nth complex roots of unity. The Nth roots of unity are given by:

$$x_k = \cos\left(\frac{2k\pi}{N}\right) + i\sin\left(\frac{2k\pi}{N}\right)$$

The sum of the Nth roots of unity is equal to 0, so

$$\sum_{j=1}^{N} \cos\left(\frac{2k\pi}{N}\right) = \sum_{j=1}^{N} \sin\left(\frac{2k\pi}{N}\right) = 0,$$

and as a result,

$$\sum_{j=1}^{N} \cos\left(\frac{2j\pi y}{N}\right) = 0$$

So, we plug in the aforementioned value of c_j.

$$\begin{aligned}
f_y(k) &= \sum_{j=1}^{N-1} c_j \sinh(\beta_j) \sin\left(\frac{j\pi k}{N}\right) \\
&= \sum_{j=1}^{N-1} \frac{2}{N} \sin\left(\frac{j\pi y}{N}\right) \sin\left(\frac{j\pi k}{N}\right).
\end{aligned}$$

If $k = y$, we get that

$$f_y(k) = \frac{2}{N}\sum_{j=1}^{N-1} \sin^2\left(\frac{j\pi k}{N}\right) = 1.$$

Earlier, we showed that the functions $\{\sin(\frac{a\pi b}{N})\}$ for $a = 1, \ldots, N-1$ are pairwise orthogonal. So, now we let $b = j$ and let $a = y$ or k, where $y \neq k$. We can do this because j, k, and y all take on values in $(1, \ldots, N-1)$. Let's consider these two functions $\sin(\frac{y\pi j}{N})$ and $\sin(\frac{k\pi j}{N})$. These two functions are then orthogonal. So, then we have

$$\sum_{j=1}^{N-1} \sin\left(\frac{j\pi y}{N}\right) \sin\left(\frac{j\pi k}{N}\right) = 0,$$

so

$$f_y(k) = \frac{2}{N}\sum_{j=1}^{N-1} \sin\left(\frac{j\pi y}{N}\right) \sin\left(\frac{j\pi k}{N}\right) = 0.$$

So, we have found that for a fixed point $(1, y) \in \partial_{1,N}$,

$$f_y(k) = \sum_{j=1}^{N-1} \frac{2}{N} \sin\left(\frac{j\pi y}{N}\right) \sin\left(\frac{j\pi k}{N}\right) = \begin{cases} 1 & \text{if } k = y \\ 0 & \text{if } k \neq y. \end{cases} \tag{5.6}$$

We now create a new function g_y:

$$g_y(x_1, x_2) = \sum_{j=1}^{N-1} \frac{2}{N \sinh(\beta_j)} \sin\left(\frac{j\pi y}{N}\right) \sinh\left(\frac{\beta_j x_1}{N}\right) \sin\left(\frac{j\pi x_2}{N}\right) \tag{5.7}$$

Notice that

$$g_y(N, x_2) = \sum_{j=1}^{N-1} \frac{2}{N} \sin\left(\frac{j\pi y}{N}\right) \sin\left(\frac{j\pi x_2}{N}\right) = \begin{cases} 1 & \text{if } k = y \\ 0 & \text{if } k \neq y. \end{cases}$$

Furthermore, because g_y is a sum of $\sinh(\frac{b_j x_1}{N})\sin(\frac{j\pi x_2}{N})$'s, and because $\sinh(\frac{b_j x_1}{N})\sin(\frac{j\pi x_2}{N})$ is harmonic on A, g_y is harmonic on A. Earlier, we showed that $\sinh\left(\frac{\beta_j x_1}{N}\right)\sin\left(\frac{j\pi x_2}{N}\right) = 0$ on $\partial_{1,0}$, $\partial_{2,0}$, and $\partial_{1,N}$, so $g_y = 0$ on these three parts.

Now, for any boundary conditions on $\partial_{1,N}$ (but still with values of 0 on $\partial_{1,0} \cup \partial_{2,0} \cup \partial_{2,N}$), we can simply take a sum of different g_y's (because the sum of harmonic equations is still harmonic). If we let $F(x)$ denote the boundary conditions on ∂A, with $F(x)$ still equal to 0 on $\partial_{1,0} \cup \partial_{2,0} \cup \partial_2 N$, the harmonic equation on A is

$$F(x_1, x_2) = \sum_{y \in (1,\ldots,N-1)} F(N, y) g_y(x_1, x_2). \tag{5.8}$$

As a side note, $[g_y(x_1, x_2)]$ is the Poisson kernel on $\partial_{1,N}$. The Poisson kernel is as follows:

$$[\mathbf{H}_A] = [H_A((x_1, x_2)(N, y))]_{(x_1,x_2)\in A,(N,y)\in\partial_{1,N}}$$

$$H_A((x_1, x_2)(N, y)) = \frac{2}{N} \sum_{j=1}^{N-1} \frac{1}{\sinh(\beta_j)} \sin\left(\frac{j\pi y}{N}\right) \sinh\left(\frac{\beta_j x_1}{N}\right) \sin\left(\frac{j\pi x_2}{N}\right).$$

6. Finite Connected Graphs With No Boundary Conditions

We will now quickly consider finite connected graphs with no boundary conditions. We can think of graphs with no boundary conditions in two ways. First, we can imagine there being no boundary points at all (that is, ∂A is empty). Or, we can still consider A and ∂A, but with the added requirement that the function is also harmonic on ∂A in addition to A.

Theorem 6.1. *The only harmonic functions on finite, connected graphs with no boundary conditions are constant functions.*

Proof. Let us choose one point x_0 on the graph A such that $F(x_0) \neq 0$. If there is no such point, then $F(x) = 0$ for all x and we are done. Then, let $F(x_0) = a$. Clearly, $F(x) = a$ for all $x \in A$ is harmonic. Assume that there is another function $G(x)$ that is harmonic on A with $G(x_0) = a$. Then, the difference of two harmonic functions is also harmonic, so $(F-G)(x)$ is also harmonic on A, and $(F-G)(x_0) = 0$.

A function that is harmonic on all $x \in A$ is clearly harmonic on $x \in A - \{x_0\}$. So, we can apply Theorem (4.1) with x_0 being a boundary condition. But, since $F(x_0) = 0$ and this is the only boundary condition,

$$(F - G)(x) = \sum_{y \in \partial A} \mathbb{P}(S_{T_A} = y | S_0 = x)(F - G)(x_0) = 0.$$

So, $F(x) = G(x)$. Therefore, the only harmonic functions on finite, connected graphs with no boundary conditions are constant functions. □

Note that this does not contradict Theorem 4.1 because that theorem deals with cases with boundary conditions. Also note that if you have a graph with A and ∂A, assign values to points on ∂A, and find the unique harmonic equation on A, if you remove ∂A, the equation is not necessarily still harmonic on A. As an example, consider the following case in $\mathbb{Z}$, where the white dots represent A and the black dots represent ∂A. The numbers below the graph represent the values of a function on $A \cup \partial A$.

1 3 5 7 9 11

This function is harmonic on A. However, if you remove ∂A, the function is no longer harmonic on A. Consider the left-most dot. Before, for the function to be harmonic, the function's value at the dot had to equal the average of the values of the two adjacent points. However, after removing ∂A, for the function to be harmonic, the value at the point now has to be the average of the one adjacent point.

3 5 7 9

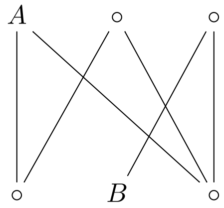
7. Harmonic Functions on Bipartite Graphs with Boundary Conditions

Definition 7.1. A graph G is *bipartite* if there exists a partition $V = V_1 \dot{\bigcup} V_2$ such that all edges go between V_1 and V_2.

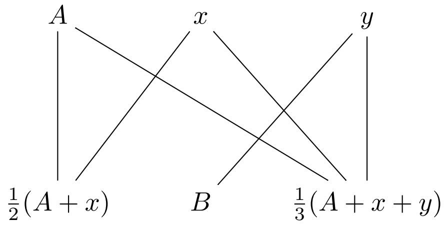
From Theorem 4.1, we know that the unique harmonic function on a specific finite, connected graph with boundary conditions is the one where

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

However, this does not give a very practical way of finding the harmonic function. One way of finding the harmonic function is by simply setting up a system of equations. First, we take V_1 and assign every vertex in that set a variable. Then, we can write what the vertices in V_2 are in terms of these variables. Then, we go back to V and create a system of equations that must be true in order for $F(x)$ to be harmonic. As an example, consider the following bipartite graph:



A and B represent the two boundary values on the graph. We label the vertices on the top section x and y and find out what the two bottom vertices must be in order for the function to be harmonic.



Then, we can set up the following system of equations:

$$x = \frac{1}{2}[\frac{1}{2}(A+x) + \frac{1}{3}(A+x+y)]$$
$$y = \frac{1}{2}[B + \frac{1}{3}(A+x+y)].$$

Solving this system of equations gets:

$$x = \frac{9A+2B}{11}$$
$$y = \frac{4A+7B}{11}.$$

8. The Heat Equation On Graphs

The paper has talked about harmonic functions on general graphs. As mentioned before, on regular graphs, if F is a function describing the heat distribution on the graph, F being harmonic means that the heat is at an equilibrium — the change in heat at every point from time n to time $n+1$ will be 0. However, this is not necessarily true for non-regular graphs.

Trying to find an equilibrium for all graphs is a more difficult question. For functions $F : V \to \mathbb{R}$, let us define two operators R and S as follows:

$$RF(x) = \sum_{y \sim x,\ y \in G} \frac{F(y)}{\deg(y)} \tag{8.1}$$

$$SF(x) = (R - I)F(x) = \sum_{y \sim x,\ y \in G} \frac{F(y)}{\deg(y)} - \frac{F(x)}{\deg(x)} \tag{8.2}$$

It is easy to see that for general graphs, $RF(x)$ describes the amount of heat flow into point x by the next time interval, and $SF(x)$ describes the change in temperature at point x. So, solving for an equilibrium when given boundary points requires finding when $SF(x)$=0.

Finding a general solution to $SF(x)$, as we did with $QF(x)$, will not be covered in this paper. However, we will consider finding a solution to this for specific finite, connected graphs.

First we will look at finite, connected graphs with no boundary conditions. To find the solution, we set up a transition matrix T for all points on the graph.

Definition 8.3. A *transition matrix* T has entries p_{ij} where

$$p_{ij} = \mathbb{P}(x_{t+1} = i | x_t = j).$$

Then, let the column matrix q_t be

$$\begin{bmatrix} q_{t_1} \\ q_{t_2} \\ \vdots \\ q_{t_n} \end{bmatrix}$$

q_t is the $n \times 1$ matrix representing the values of $f(x)$ at time t. For a bipartite graph, there are a few things to note about the transition matrix. First, if $i \in V_1$ and $j \in V_1$, or if $i \in V_2$ and $j \in V_2$, then $p_{ij} = 0$. Also, if $i \sim j$, then $p_{ij} = \frac{1}{\deg(j)}$. Notice that the transition matrix for a graph is very similar to the adjacency matrix, which we will define:

Definition 8.4. An *adjacency matrix* A has entries p_{ij} where

$$p_{ij} = \begin{cases} 1 & \text{if } i \sim j \\ 0 & \text{if } i \not\sim j \end{cases}$$

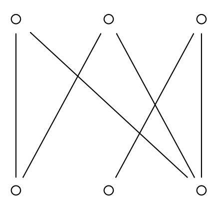
In fact, the transition matrix for graphs with no boundary conditions is

$$p_{ij} = \begin{cases} \frac{1}{\deg(j)} & \text{if } i \sim j \\ 0 & \text{if } i \not\sim j \end{cases}$$

Consider what happens when you multiply T by q_t. In the resulting matrix $n \times 1$ matrix, each element corresponding to a point i is equal to

$$\sum_{i \sim j,\ j \in G} \frac{1}{\deg(j)} \cdot F(j) + \sum_{i \not\sim j,\ j \in G} 0 \cdot F(j) = RF(i).$$

To find the stationary distribution q, we let $T \cdot q_t = q_t$ and solve the resulting system of equations. As an example, consider the following bipartite graph.



If we number across from left to right on the upper row and then left to right on the lower row, the adjacency matrix A looks like

$$\begin{bmatrix} 0 & 0 & 0 & 1 & 0 & 1 \\ 0 & 0 & 0 & 1 & 0 & 1 \\ 0 & 0 & 0 & 0 & 1 & 1 \\ 1 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 \\ 1 & 1 & 1 & 0 & 0 & 0 \end{bmatrix}$$

and the transition matrix T looks like

$$\begin{bmatrix} 0 & 0 & 0 & \frac{1}{2} & 0 & \frac{1}{3} \\ 0 & 0 & 0 & \frac{1}{2} & 0 & \frac{1}{3} \\ 0 & 0 & 0 & 0 & 1 & \frac{1}{3} \\ \frac{1}{2} & \frac{1}{2} & 0 & 0 & 0 & 0 \\ 0 & 0 & \frac{1}{2} & 0 & 0 & 0 \\ \frac{1}{2} & \frac{1}{2} & \frac{1}{2} & 0 & 0 & 0 \end{bmatrix}.$$

We let the stationary distribution matrix q be

$$\begin{bmatrix} x_1 \\ x_2 \\ x_3 \\ x_4 \\ x_5 \\ x_6 \end{bmatrix}$$

and set $T \cdot q = q$ and solve the resulting system of equations.

In this case, the solutions are of the form

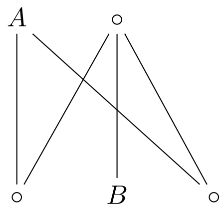
$$\begin{bmatrix} x_1 \\ x_1 \\ x_1 \\ x_1 \\ x_1/2 \\ 3x_1/2 \end{bmatrix}$$

If there are boundary conditions,we need to define T differently than we did for graphs without boundary conditions. We define T as

$$p_{ij} = \begin{cases} \frac{1}{j} & \text{if } i \sim j \text{ and } i \in A \\ 1 & \text{if } i = j \text{ and } i \in \partial A \\ 0 & \text{if } (i \neq j \text{ and } i \in \partial A) \text{ or } (i \not\sim j \text{ and } i \in A) \end{cases}$$

For points in A, $RF(x)$ is defined as before. However, the values of the boundary points remain constant, so if $i \in \partial A$, $p_{ij} = 1$ only if $i = j$.

To solve for a specific case, set $T \cdot q = q$ and solve the resulting system of equations. For example, consider the following bipartite graph with the boundary conditions denoted by A and B.



Then, T is equal to

$$\begin{bmatrix} 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & \frac{1}{2} & 1 & \frac{1}{2} \\ \frac{1}{2} & \frac{1}{3} & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 \\ \frac{1}{2} & \frac{1}{3} & 0 & 0 & 0 \end{bmatrix}$$

and we let q be

$$\begin{bmatrix} A \\ x_1 \\ x_2 \\ B \\ x_3 \end{bmatrix}.$$

Once again we take $T \cdot q = q$ and solve for q. The solution is

$$\begin{bmatrix} A \\ (3A+6B)/4 \\ (3A+2B)/4 \\ B \\ (3A+2B)/4 \end{bmatrix}.$$

We can show that the solution for a graph with fixed boundary conditions is unique. From the definition of $RF(x)$, it is easy to see that if $RF_1(x) = 0$ and $RF_2(x) = 0$, then $R(F_1 - F_2)(x) = 0$. Then, we look at $(F_1 - F_2)(x)$ and note that $(F_1 - F_2)(x) = 0$ for $x \in \partial A$. If $F(x) = 0$ for all $x \in \partial A$, then $F(x) = 0$ for all $x \in A$. Therefore, $F_1(x) = F_2(x)$.

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