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Discrete Green's Functions

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We study discrete Green's functions and their relationship with discrete Laplace equations. Several methods for deriving Green's functions are discussed. Green's functions can be used to deal with diffusion-type problems on graphs, such as chip-firing, load balancing, and discrete Markov chains.

1. INTRODUCTION

Many combinatorial problems involve solving equations of the following general type. Let V denote a set of states (in the setting of Markov chains) or a set of vertices (as in a graph). Let g denote a given function $g\colon V \to \mathbb{R}$. The problem of interest is to find f satisfying the following discrete Laplace equation,

$$\Delta f(x) = \sum_y (f(x) - f(y))\, p_{xy} = g(x), \tag{1}$$

where p_{xy} denote the transition probability from x to y. For a typical random walk in a graph, p_{xy} is often taken to be $1/d_x$ for y adjacent to x and 0 otherwise (where d_x is the degree of x).

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For some combinatorial games or diffusion processes, there are additional constraints for finding solutions f in (1). For a subset S of V, we define the *boundary* δS of S by

$$\delta S = \{ y \notin S : p_{xy} \neq 0 \text{ for some } x \in S \}.$$

For a function $\sigma : \delta S \to \mathbb{R}$, we say f satisfies the boundary condition σ if $f(x) = \sigma(x)$ for x in δS.

For example, the problem of evaluating the probability $f_{x,y}(z)$ of a Markov chain hitting x before hitting y can be formulated as the following problem of solving the Laplace equation with boundary conditions. We consider $S = V - \{x, y\}$, $\delta S = \{x, y\}$ and $\sigma(x) = 1$, $\sigma(y) = 0$. Then $f_{x,y}(z)$ is the solution for the following equation,

$$\Delta f(z) = 0,$$

for all $z \in S$ and f satisfies the boundary condition σ.

Suppose $\delta S \neq \emptyset$ and the subgraph induced by S is connected. It is not hard to see [6] that Δ is nonsingular as an operator on the space of functions defined on S. The Green's function is the left inverse operator of the Laplace operator Δ (restricted to the subspace of functions defined on S):

$$G\Delta = I,$$

where I is the identity operator.

If we can determine the Green's function G, then we can solve the Laplace equation in (1) by writing

$$f = G\,\Delta f = Gg.$$

We will also consider Green's functions for the case that there is no boundary. We will discuss a related example which concerns the so-called "hitting time," the expected number of steps for a Markov chain to reach a state y with initial state x. It is worth mentioning that numerous diffusion-type problems can be treated in a similar way, including chip-firing games, load balancing algorithms, and the mixing of random walks. Thus, Green's functions provide a powerful tool in dealing with a wide range of combinatorial problems.

Green's functions were introduced in a famous essay by George Green [16] in 1828 and have been extensively used in solving differential equations [2, 5, 15]. The concept of Green's functions has been used in numerous areas. Many formulations of Green's functions are given on a variety of topics. Articles on discrete Green's functions or discrete analytic functions appear sporadically in the literature, most of which concern either discrete regions of a manifold or finite approximations of the equations [3, 12, 17, 13, 19, 21]. In this paper, we consider Green's functions for discrete Laplace equations.

This paper is organized as follows: In Section 2, we will give some basic definitions of Dirichlet eigenvalues and heat kernels. In Section 3, we derive an explicit formula for Green's functions in terms of Dirichlet eigenfunctions. In Section 4, we will consider some direct methods for deriving Green's functions for paths. In Section 5, we consider a general form of Green's function which can then be used to solve for Green's functions for lattices. In Section 6, we will evaluate Green's functions for several families of graphs including distance regular graphs. In Section 7, we consider Green's functions for the boundaryless case and discuss its relationships to the problem of expected hitting time.

2. DIRICHLET EIGENVALUES AND THE HEAT KERNEL

We consider a reversible Markov chain (p_{xy}) which can also be viewed as a weighted undirected graph with edge weights w_{xy} (with $w_{xy} = p_{xy}\pi(x)$ where π is the stationary distribution). We will first give some basic definitions for a normalized Laplacian and for heat kernels with Dirichlet boundary conditions.

The discrete Laplace operator as defined in (1) is not a self-adjoint operator. The corresponding matrix, also denoted by Δ, has entries

$$\Delta(x, y) = \begin{cases} 1 - w_{x,x}/d_x & \text{if} \quad x = y \text{ and } d_x \neq 0, \\ -w_{x,y}/d_x & \text{if} \quad x \text{ and } y \text{ are adjacent}, \\ 0 & \text{otherwise}, \end{cases}$$

where the degree d_x of x is the sum of all $w_{x,y}$. We will assume here that $d_x \neq 0$ for all x to avoid degenerated cases. Clearly, Δ is not a symmetric matrix in general. However, Δ is equivalent to the following matrix $\mathcal{L}$,

$$\begin{aligned} \mathcal{L} &= T^{1/2} \Delta T^{-1/2} \\ &= T^{-1/2} L T^{-1/2}, \end{aligned}$$

where T is a diagonal matrix with entries $T(x, x) = d_x$ and L is the combinatorial Laplacian:

$$L(x, y) = \begin{cases} d_x - w_{x,x} & \text{if} \quad x = y, \\ -w_{x,y} & \text{if} \quad x \text{ and } y \text{ are adjacent}, \\ 0 & \text{otherwise}. \end{cases}$$

It is easy to see that $\mathcal{L}$ is a symmetric matrix and we call $\mathcal{L}$ the *normalized* Laplacian. In this paper, we consider graphs without isolated vertices so that the d_x are all nonzero.

For a subset S of vertices, the Dirichlet eigenvalues of $\mathcal{L}$ are exactly the eigenvalues of the submatrix $\mathcal{L}_S$ with rows and columns restricted to those indexed by vertices in S. Let $\lambda_1 \leqslant \lambda_2 \leqslant \cdots \leqslant \lambda_s$ denote the eigenvalues of $\mathcal{L}_S$, where $s = |S|$. It is not hard to check (also see [6]) that

$$\begin{aligned} \lambda_1 &= \inf_g \frac{\langle g, \mathcal{L}_S g\rangle}{\langle g, g\rangle} \\ &= \inf_f \frac{\sum_{x,\, y \in S \cup \delta S} (f(x) - f(y))^2 w_{xy}}{\sum_S f^2(x)\, d_x}, \end{aligned} \tag{2}$$

where f and g range over all nontrivial functions satisfying the Dirichlet boundary condition

$$f(x) = 0 = g(x) \tag{3}$$

for all x in the boundary δS of S.

We remark that the celebrated matrix-tree theorem [18] states that the number of spanning trees in a graph Γ is equal to the determinant of L_S, where S is any maximum proper subset of the vertex set. Therefore the number of spanning trees in a graph Γ is exactly

$$\prod_{i=1}^{s} \lambda_i \prod_{x \in S} d_x.$$

We also note that in Eq. (2) the degrees d_x are the degrees in the host graph Γ (not in the induced subgraph S). When the induced subgraph S is connected, we see from (2) that $\mathcal{L}_S$ is nonsingular and $\lambda_1 > 0$ (also see [6]). Thus the inverse of $\mathcal{L}_S$, denoted by $\mathcal{G}$, is well defined. We note that $\mathcal{G}$ is just a symmetric normalized version of the Green's function G since

$$\mathcal{G} = T^{1/2} G T^{-1/2}$$

and we have

$$T^{-1/2} \mathcal{G} T^{1/2} \Delta = 0.$$

For example, suppose we consider a path P_n which can be regarded as an induced subgraph of a cycle C_m, with $m > n+1$. Suppose that the vertices of P_n are 1, 2, ..., n where the boundary consists of two vertices 0 and $n+1$. Then

$$\Delta f(x) = \tfrac{1}{2}(2f(x) - f(x-1) - f(x+1))$$

and $\Delta = \mathscr{L} = \frac{1}{2}L$ since $d_x = 2$ for all x. The Dirichlet eigenvalues for P_n are $1 - \cos \frac{k\pi}{n+1}$ and the corresponding eigenfunctions are

$$\phi_k(j) = \sqrt{\frac{2}{n+1}} \sin \frac{jk\pi}{n+1}$$

for $k = 1, ..., n$. The problem of determining the Green's function G for a path will be discussed later.

For a given connected induced subgraph S of a graph Γ, and for a real parameter $t \geqslant 0$, the Dirichlet heat kernel of S is defined by

$$\mathscr{H}_t(x, y) = \sum_{i=1}^{s} e^{-\lambda_i t} \phi_i(x)\, \phi_i(y), \tag{4}$$

where λ_i's are the eigenvalues of $\mathscr{L}_S$ and ϕ_i's are the corresponding orthonormal eigenfunctions. It follows from the definition (2.4) that $\mathscr{H}_t$ satisfies the following heat equation,

$$\frac{d}{dt} \mathscr{H}_t f = -\mathscr{L}_S f, \tag{5}$$

for any f satisfying the Dirichlet boundary condition. Furthermore, we have $\mathscr{H}_0 = I$ and

$$\lim_{t \to \infty} \mathscr{H}_t(x, y) = 0. \tag{6}$$

We can write

$$\begin{aligned} \mathscr{H}_t &= e^{-t\mathscr{L}_S} \\ &= I - t\mathscr{L}_S + \frac{t^2}{2!} \mathscr{L}^2 + \cdots. \end{aligned}$$

Let $\mathscr{A} = I - \mathscr{L}_S$ satisfy

$$\mathscr{A}(x, y) = \frac{w_{xy}}{\sqrt{d_x d_y}}.$$

We can express $\mathscr{H}_S$ in an alternative form,

$$\begin{aligned}\mathscr{H}_t &= e^{-t} e^{t\mathscr{A}} \\ &= e^{-t}\left(I + t\mathscr{A} + \frac{t^2}{2!}\mathscr{A} + \cdots\right) \\ &= e^{-t} \sum_{k \geqslant 0} P_k(x, y)\frac{t^k}{k!},\end{aligned}$$

where $P_k(x, y)$ is the sum of the weights of all paths of length k joining x and y. Here, the weight of a path is the product of all edge weights in the path. We use the convention that $P_0(x, x) = 1$.

We consider G satisfying

$$G\,\Delta h = h \tag{7}$$

for any h which satisfies the Dirichlet boundary condition as in (3).

In other words, (7) is equivalent to solving for G the equation

$$G\Delta_S = I_S, \tag{8}$$

where all G, Δ_S, and I_S are matrices with rows and columns indexed by elements in S.

We observe that solving for G in (8) is also equivalent to finding a symmetric matrix $\mathscr{G} = T^{1/2} G T^{-1/2}$ which satisfies the corresponding equation:

$$\mathscr{G}\mathscr{L}_S = I_S = \mathscr{L}\mathscr{G}_S. \tag{9}$$

Therefore, for a connected graph, we have the following formula for the Green function,

$$\mathscr{G}(x, y) = \sum_i \frac{1}{\lambda_i}\,\phi_i(x)\,\phi_i(y), \tag{10}$$

where ϕ_i's are orthonormal eigenfunctions with associated eigenvalues λ_i. Let $\mathscr{H}$ denote the Dirichlet heat kernel for a connected induced subgraph S. Then we have

$$\mathscr{G} = \int_0^\infty \mathscr{H}_t\, dt \tag{11}$$

since $\int_0^\infty e^{-t\lambda}\,dt = 1/\lambda_i$. And the Green's function G satisfies

$$G(x, y) = \int_0^\infty d_x^{1/2}\,\mathscr{H}_t(x, y)\,d_y^{-1/2}\,dt \tag{12}$$

$$= \sum_i \frac{1}{\lambda_i}\,d_x^{1/2}\phi_i(x)\,\phi_i(y)\,d_y^{-1/2} \tag{13}$$

for x, y in S.

3. SOLVING THE LAPLACE EQUATION USING DIRICHLET EIGENFUNCTIONS

For a connected induced subgraph S, we want to solve for f satisfying

$$\Delta f = g$$

for given g defined on $S \cup \delta S$. There are two main steps for deriving a solution f. In this section, we deal with the first part of finding a solution to $\Delta f = 0$ satisfying the boundary condition σ, a function defined on the boundary δS.

THEOREM 1. *We consider a solution f to the following equation*

$$\Delta f(x) = 0$$

for all $x \in S$ satisfying the boundary condition

$$f(y) = \sigma(y)$$

for $y \in \delta S$. Then f can be written as

$$f(z) = \sum_i \left(\frac{1}{\lambda_i} \sum_{\substack{x \in S \\ x \sim y \in \delta S}} \sqrt{d_x}\,\phi(x)\,\sigma(y) \right) d_z^{-1/2}\phi_i$$

for z in S where ϕ_i's are the eigenfunctions of $\mathscr{L}_S$.

Proof. We consider $\tilde{f}(x) = T^{1/2} f(x)$ and $\tilde{f}\colon S \to \mathbb{R}$ is the solution of the following equation,

$$\mathscr{L}_S\,\tilde{f}(x) = 0,$$

for $x \in S$. We can write $\tilde{f}$ as a linear combination of the eigenfunctions ϕ_i of $\mathscr{L}_S$.

$$\tilde{f} = \sum_i a_i \phi_i ,$$

which implies

$$a_i = \langle \phi_i, \tilde{f} \rangle.$$

Now we consider the function

$$f_0(x) = \begin{cases} 0 & \text{if } x \in S, \\ \sigma(x) & \text{otherwise.} \end{cases}$$

Let f_S denote the function f restricted to S. Clearly, $f - f_0$ satisfies the Dirichlet boundary condition. We have

$$\begin{aligned}
\lambda_i a_i &= \langle \mathscr{L}_S \phi_i, \tilde{f} \rangle \\
&= \langle \mathscr{L}_S \phi_i, (\tilde{f} - \tilde{f}_0) \rangle \\
&= \langle \phi_i, T^{-1/2} L T^{-1/2} (\tilde{f} - \tilde{f}_0) \rangle \\
&= \langle \phi_i, T^{-1/2} L (f - f_0)_S \rangle \\
&= \langle T^{1/2} \phi_i, \Delta (f - f_0)_S \rangle \\
&= \langle T^{1/2} \phi_i, -(\Delta f_0)_S \rangle \\
&= -\sum_{x \in S} \sqrt{d_x} \phi_i(x) \frac{1}{d_x} \sum_{y \sim x} (f_0(x) - f_0(y)) \\
&= \sum_{x \in S} \sum_{\substack{y \in x \\ y \in \delta S}} d_x^{-1/2} \phi_i(x) \sigma(y).
\end{aligned}$$

Consequently,

$$a_i = \frac{1}{\lambda_i} \sum_{\substack{x \in S \\ x \sim y \in \delta S}} d_x^{-1/2} \phi_i(x) \sigma(y)$$

$$\tilde{f} = \sum_i \left(\frac{1}{\lambda_i} \sum_{\substack{x \in S \\ x \sim y \in \delta S}} d_x^{-1/2} \phi_i(x) \sigma(y) \right) \phi_i$$

and so

$$f_S(z)=\sum_i \left(\frac{1}{\lambda_i} \sum_{\substack{x\in S\\ x\sim y\in \delta S}} d_x^{-1/2}\phi_i(x)\,\sigma(y)\right) d_z^{-1/2}\phi_i(z).$$

This completes the proof of Theorem 1. ∎

EXAMPLE 1. For a path P_n with vertex set $\{1, 2, ..., n\}$, we assume the boundary condition $\sigma(n+1)=0$ and $\sigma(0)=1$. The solution $f(x)$ to the equation $\Delta f=0$ satisfying the boundary condition σ is the probability of a walk starting from x hitting 0 before hitting $n+1$. We can solve for f directly and get

$$f(z)=1-\frac{z}{n+1}.$$

On the other hand, by Theorem 1, f can be found as follows:

$$\tilde{f}(z)=f(z)\,d_z^{1/2}$$
$$=\sum_k a_k\phi_k,$$

$$\text{where } a_k=\frac{1}{1-\cos\frac{k\pi}{n+1}}\,\frac{\sin\frac{k\pi}{n+1}}{\sqrt{n+1}}.$$

Therefore, for $z=1, ..., n$, we have

$$f(z)=\frac{1}{n+1}\sum_{k=1}^{n}\frac{\sin\frac{k\pi}{n+1}\sin\frac{kz\pi}{n+1}}{1-\cos\frac{k\pi}{n+1}}$$
$$=1-\frac{z}{n+1}$$

which is the probability that a random walk starting from z hits 0 before it hits $n+1$.

A solution to the Laplace equation (1) can be described in a general form:

THEOREM 2. *In a connected induced subgraph S of a graph Γ, let g denote a function $g\colon S \to \mathbb{R}$ and let σ denote a boundary condition $\sigma\colon \delta S \to \mathbb{R}$. A solution f to the Laplace equation*

$$\Delta f(x) = g(x)$$

for $x \in S$ and for $y \in \delta S$,

$$f(y) = \sigma(y)$$

can be written as

$$f = f_1 + f_2,$$

where f_1 is a solution to $\Delta f_1(x) = 0$ which satisfies the boundary condition σ, and f_2, which satisfies the Dirichlet boundary condition, is defined by

$$f_2 = Gg.$$

The proof is immediate. We can use Theorem 1 to determine f_1. The evaluation for f_2 depends on the Green's function. Various methods for determining the Green's function will be discussed in the next section.

4. GREEN'S FUNCTION FOR A PATH

In the previous sections, we have given several explicit formulas for the Green's function. Here, however, we consider direct methods for evaluating the Green's function for a path with Dirichlet boundary condition. The solutions we will obtain lead to some intriguing equalities.

Let the vertex set of P_n be denoted by $\{1, 2, ..., n\}$ with boundary $\{0, n+1\}$. Since $\Delta = \mathcal{L} = L/2$, we have $\mathcal{L}G = G\mathcal{L} = I$. Here we assume $1 \leqslant x < y \leqslant n$. From $\mathcal{L}G = I$, it follows that

$$\tfrac{1}{2}(2G(x, y) - G(x-1, y) - G(x+1, y)) = 0.$$

From $G\mathcal{L} = I$, we have

$$\tfrac{1}{2}(2G(x, y) - G(x, y-1) - G(x, y+1)) = 0.$$

Here we use the convention that $G(x, y) = 0$ if either x or y is not in $\{1, ..., n\}$. Therefore we have

$$\begin{aligned} G(x, y) - G(x-1, y) &= G(x-1, y) - G(x-2, y) \\ &= G(x-2, y) - G(x-3, y) \\ &= \cdots \\ &= G(1, y). \end{aligned}$$

This implies that

$$G(x, y) = xG(1, y).$$

In a similar way, we can get

$$G(1, y) = c(n+1-y)$$

for some constant c. Now, we use the fact that

$$\tfrac{1}{2}(2G(x, x) - G(x-1, x) - G(x+1, x)) = 1$$

to get $c = \frac{2}{n+1}$ and $G(x, x) = cx(n+1-x)$. Thus we have proved the following:

THEOREM 3. *For a path P_n with vertex set $\{1, ..., n\}$ as an induced subgraph with boundary $\{0, n+1\}$, its Green's function satisfies*

$$G(x, y) = \frac{2}{n+1}\, x(n+1-y)$$

for $1 \leqslant x \leqslant y \leqslant n$.

As an immediate consequence of Theorem 3 and Eq. (10), we obtain the following (somewhat nontrivial) equality:

COROLLARY 1. *The following equality holds for integers $1 \leqslant x \leqslant y \leqslant n$:*

$$\sum_{k=1}^{n} \frac{\sin \dfrac{kx\pi}{n+1} \sin \dfrac{ky\pi}{n+1}}{1 - \cos \dfrac{k\pi}{n+1}} = x(n+1-y).$$

5. GREEN'S FUNCTIONS FOR LATTICES

In this section, we describe a way to determine Green's functions for the Cartesian product of graphs. In particular, this method can be used to evaluate Green's functions for lattices.

We start with an induced subgraph S of a graph Γ. For $\alpha \in \mathbb{R}$, let $\mathcal{G}_\alpha$ denote the symmetric matrix satisfying

$$(\mathcal{L}_S + \alpha)\, \mathcal{G}_\alpha = I_S,$$

where $\mathcal{L}_S$ is the Dirichlet Laplacian for the induced subgraph S. Clearly,

$$\mathcal{G}_\alpha(x, y) = \sum_i \frac{1}{\lambda_i + \alpha}\, \phi_i(x)\, \phi_i(y),$$

where ϕ_i's are orthonormal eigenfunctions of $\mathcal{L}_S$ associated with eigenvalues λ_i.

Now we consider two induced subgraphs S and S' of graphs Γ and Γ', respectively. We let $S \times S'$ denote the induced subgraph of the Cartesian product of Γ and Γ' by the subset of vertices (v, v') where $v \in S$ and $v' \in S'$. The Cartesian product of two graphs (V, E) and (V', E') has vertex set $\{(v, v') : v \in V, v' \in V'\}$ and edges of the form $\{(v, v'), (v, u')\}$ or $\{(v, v'), (u, v')\}$ where $\{u, v\} \in E$, $\{u', v'\} \in E'$.

Let C denote a contour in the plane, say, consisting of all $\alpha \in \mathbb{C}$ satisfying $|2 - \alpha| = 2$.

Let $\mathcal{G}$ and $\mathcal{G}'$ denote the Green's functions of S and S', respectively. Then we have the following:

THEOREM 4. *Suppose S and S' are induced subgraphs of two graphs Γ and Γ', which are both regular of degrees d. The Green's function* **G** *of the cartesian product $S \times S'$ with Dirichlet boundary condition is*

$$\mathbf{G}((x, x'), (y, y')) = \frac{1}{\pi i} \int_C \mathcal{G}_\alpha(x, y)\, \mathcal{G}'_{-\alpha}(x', y')\, d\alpha,$$

where C, $\mathcal{G}$, $\mathcal{G}'$ are defined as above.

Proof. Let ϕ_j and ϕ'_k denote the eigenfunctions of the Laplacian $\mathcal{L}_S$ and $\mathcal{L}_{S'}$, with eigenvalues λ_j and λ'_k, respectively. The eigenvalues of $S \times S'$ are $(\lambda_j + \lambda'_k)/2$. We see that

$$\mathbf{G}((x, x'), (y, y')) = 2 \sum_{j, k} \frac{\phi_j(x)\, \phi_k(y)\, \phi_j'(x')\, \phi_k(y')}{\lambda_j + \lambda_k'}$$

$$= \frac{1}{\pi i} \int_C \sum_{j, k} \frac{\phi_j(x)\, \phi_k(y)\, \phi_j'(x')\, \phi_k(y')}{(\lambda_j + \alpha)(\lambda_k' - \alpha)}\, d\alpha$$

$$= \frac{1}{\pi i} \int_C \mathcal{G}_\alpha(x, y)\, \mathcal{G}'_{-\alpha}(x', y')\, d\alpha. \quad \blacksquare$$

We can use the same method to obtain a formulation for the following general Cartesion product of two graphs.

THEOREM 5. *Suppose S and S' are induced subgraphs of two graphs Γ and Γ', which are regular of degrees d and d', respectively. The Green's function* $\mathbf{G}$ *of the Cartesian product $S \times S'$ with Dirichlet boundary condition is*

$$\mathbf{G}((x, x'), (y, y')) = \frac{d + d'}{2\pi i\, dd'} \int_C \mathcal{G}_{\alpha/d}(x, y)\, \mathcal{G}'_{-\alpha/d'}(x', y')\, d\alpha,$$

where C is a contour consisting of all $\alpha \in \mathbb{C}$ satisfying $|d + d' - \alpha| = d + d'$.

Proof. Let ϕ_j and ϕ_k' denote the eigenfunctions of the Laplacian $\mathcal{L}_S$ and $\mathcal{L}_{S'}$, with eigenvalues λ_j and λ_k', respectively. The eigenvalues of $S \times S'$ are

$$\frac{d}{d + d'}\, \lambda_j + \frac{d'}{d + d'}\, \lambda_k'. \quad \blacksquare$$

We now consider the two dimensional lattice graph $P_m \times P_n$ with vertex set $\{(x, y) : 1 \leqslant x \leqslant m, 1 \leqslant y \leqslant n\}$ and edges of the form $\{(x, y), (x + 1, y)\}$ and $\{(x, y), (x, y + 1)\}$.

THEOREM 6. *The lattice graph $P_m \times P_n$ has Green's function*

$$G((x, x'), (y, y')) =$$

$$\sum_{k=1}^{n} \frac{8(-1)^{k-1} \sin \frac{\pi k x'}{n+1} \sin \frac{\pi k y'}{n+1}\, U_{x-1}\left(2 - \cos \frac{\pi k}{n+1}\right) U_{m-y}\left(2 - \cos \frac{\pi k}{n+1}\right)}{(n+1)\, U_m\left(2 - \cos \frac{\pi k}{n+1}\right)},$$

where U_n is the Chebyshev polynomial of the second kind.

Its proof needs the following useful fact:

THEOREM 7. *For a path P with vertices $1, 2, ..., n$ and a real α, the Green's function G_α satisfies*

$$G_\alpha(x, y) = \frac{2(r^x - r^{-x})(r^{n+1-y} - r^{-(n+1-y)})}{(r - r^{-1})(r^{n+1} - r^{-(n+1)})},$$

where $2(1+\alpha) = r + r^{-1}$.

Proof. For $\alpha = 0$, we know from Theorem 3 that $G_0(x, y) = 2x(n+1-y)/(n+1)$. For $x < y$, we have

$$\begin{aligned} 0 &= (\mathscr{L} + \alpha)\, G_\alpha(x, y) \\ &= \tfrac{1}{2}(2(1+\alpha)\, G_\alpha(x, y) - G_\alpha(x+1, y) - G_\alpha(x-1, y)) \\ &= \tfrac{1}{2}((r + r^{-1})\, G_\alpha(x, y) - G_\alpha(x+1, y) - G_\alpha(x-1, y)). \end{aligned}$$

This implies

$$\begin{aligned} G_\alpha(x+1, y) - rG_\alpha(x, y) &= \frac{1}{r}\,(G_\alpha(x, y) - rG_\alpha(x-1, y)) \\ &= \cdots \\ &= \frac{c_y}{r^x}. \end{aligned}$$

For $x \leqslant y$, we have

$$\begin{aligned} G_\alpha(x, y) &= \frac{c_y}{r^{x-1}} + rG(x-1, y) \\ &= \frac{c_y}{r^{x-1}}\,(1 + r^2 + \cdots + r^{2(x-1)}) \\ &= \frac{c'_y(r^{2x} - 1)}{r^{x-1}}. \end{aligned}$$

In a similar way, we get

$$G_\alpha(x, y) = c(r^{2x} - 1)(1 - r^{-2(n+1-y)})\, r^{-x-y}.$$

To determine the value of c, we consider

$$
\begin{aligned}
1 &= (\mathscr{L}+\alpha)\, G(x,x) \\
&= \frac{1}{2}\left((r+r^{-1})\, G(x,x) - G(x+1,x) - G(x-1,x)\right) \\
&= \frac{c}{2}\Bigg(\frac{(r+r^{-1})(r^{2x}-1)(1-r^{-2(n+1-x)})}{r^{2x}} \\
&\qquad - \frac{(r^{2x}-1)(1-r^{-2(n-x)})}{r^{2x+1}} - \frac{(r^{2(x-1)}-1)(1-r^{-2(n+1-x)})}{r^{2x-1}}\Bigg) \\
&= \frac{c}{2}\left(\frac{r^{2x}(1-r^{-2})(1-r^{-2(n+1-x)})}{r^{2x-1}} + \frac{(r^{2x}-1)(-1+r^{2})\, r^{-2(n+1-x)}}{r^{2x+1}}\right) \\
&= \frac{c}{2}\,\frac{(r^2-1)(r^{2x}(1-r^{-2(n+1-x)}) + r^{-2(n+1-x)}(r^{2x}-1))}{r^{2x+1}} \\
&= \frac{c}{2}\,\frac{(r^2-1)(r^{2x}-r^{-2(n+1-x)})}{r^{2x+1}} \\
&= \frac{c}{2}\,\frac{(r^2-1)(1-r^{-2(n+1)})}{r}.
\end{aligned}
$$

This implies

$$
c = \frac{2r}{(r^2-1)(1-r^{-2(n+1)})}.
$$

Thus we have

$$
\begin{aligned}
G_\alpha(x,y) &= \frac{2(r^{2x}-1)(1-r^{-2(n+1-y)})}{(r-r^{-1})(1-r^{-2(n+1)})\, r^{x+y}} \\
&= \frac{2(r^{x}-r^{-x})(r^{n+1-y}-r^{-(n+1-y)})}{(r-r^{-1})(r^{n+1}-r^{-(n+1)})}
\end{aligned}
$$

as claimed. ∎

By using the above theorem and the definitions of α, r, we have the following:

COROLLARY 2. *For a real* $\alpha \neq 0$, *the Green's function* G_α *for a path* P *with vertices* 1, 2, ..., n *satisfies*

$$G_\alpha(x, y) = \frac{2U_{x-1}(1+\alpha)\, U_{n-y}(1+\alpha)}{U_n(1+\alpha)},$$

where U *is the Chebyshev polynomial of the second kind.*

Now we are ready to prove Theorem 6.

Proof of Theorem 6. From Theorem 4, it is enough to determine the residues of $G_\alpha(x, y)\, G'_{-\alpha}(x', y')$ for α in the interior of the contour C. From Theorem 7, the poles of $G_\alpha G'_{-\alpha}$ are exactly at $r = e^{i\pi k/(n+1)}$ satisfying $1 - r^{-2(n+1)} = 0$. This implies

$$\alpha = 1 - \cos \frac{\pi k}{n+1}.$$

The residue of $G'_{-\alpha}(x', y')$ at $\alpha = 1 - \cos \frac{\pi k}{n+1}$ is exactly

$$\frac{(-1)^{k-1} \sin \dfrac{\pi k x'}{n+1} \sin \dfrac{\pi k y'}{n+1}}{n+1}.$$

Therefore the Green's function of $P_m \times P_n$ satisfies

$$G((x, x'), (y, y')) = 2\, Res\, G_\alpha(x, y)\, G'_{-\alpha}(x', y')$$

$$= \sum_{k=1}^{n} \frac{8(-1)^{k-1} \sin \dfrac{\pi k x'}{n+1} \sin \dfrac{\pi k y'}{n+1}\, U_{x-1}\left(2 - \cos \dfrac{\pi k}{n+1}\right) U_{m-y}\left(2 - \cos \dfrac{\pi k}{n+1}\right)}{(n+1)\, U_m\left(2 - \cos \dfrac{\pi k}{n+1}\right)} \quad \blacksquare$$

By combining Theorem 6 and Eq. (10), we have the following:

COROLLARY 3.

$$\frac{1}{m+1} \sum_{k=1}^{m} \sum_{j=1}^{n} \frac{\sin \dfrac{k\pi x}{m+1} \sin \dfrac{k\pi y}{m+1} \sin \dfrac{j\pi x'}{n+1} \sin \dfrac{j\pi y'}{n+1}}{2 - \cos \dfrac{\pi k}{m+1} \cos \dfrac{\pi j}{n+1}}$$

$$= \sum_{k=1}^{n} \frac{(-1)^{k-1} \sin \dfrac{\pi k x'}{n+1} \sin \dfrac{\pi k y'}{n+1}\, U_{x-1}\left(2 - \cos \dfrac{\pi k}{n+1}\right) U_{m-y}\left(2 - \cos \dfrac{\pi k}{n+1}\right)}{U_m\left(2 - \cos \dfrac{\pi k}{n+1}\right)}$$

6. GREEN'S FUNCTIONS FOR DISTANCE REGULAR GRAPHS

For two vertices in a graph, the *distance* is the number of edges in a shortest path joining the two vertices. A graph Γ is said to be *distance regular* if for any two vertices x and y of distance k in Γ, the number of neighbors of y of distance $k-1$, k, $k+1$ from x respectively, are constants depending only on k (and independent of the choice of x and y). In other words, a graph Γ is distance regular if Γ is a strong regular covering of a weighted path P (see [11, 14]). For a fixed vertex x, there is a natural mapping π that maps a vertex y of distance k to x in Γ to vertex v_k in P. The weight of an edge $\{v_k, v_{k+1}\}$ in P is the sum of all edge weights $w(y, z)$ in Γ where $\pi(y) = v_k$ and $\pi(z) = v_{k+1}$. It is not difficult to check that all eigenvalues of Γ are eigenvalues of P. Furthermore, the multiplicities of eigenvalues in Γ can be determined by the eigenfunctions of P. The heat kernel $\mathscr{H}$ of Γ and the heat kernel h of P are related in a nice way [11]:

$$\mathscr{H}_t(x, y) = \sqrt{\pi^{-1}(v_r)}\, h_t(v_0, v_r).$$

Thus Green's functions for distance regular graphs can be deduced from Green's functions for a weighted path.

We will treat a general weighted path which can then be used to deal with distance regular graphs. We consider a general weighted path with edge weights $w_{k,k+1} = w(v_k, v_{k+1})$, for $k = 0, ..., m$. We will consider two situations with respect to the boundary. (The case with no boundary will be examined in Section 7.) In the first case the boundary consists of one single vertex v_0. In the second case the boundary is $\{v_0, v_{m+1}\}$. As a matter of fact, the first case can be viewed as a special case of the second in the sense that the edge weight of the last edge $w_{m-1,m}$ is zero, although the Green's functions for two cases are quite different.

6.1. *The Boundary Has One Single Vertex*

In this subsection, we consider the Green's function G with Dirichlet boundary condition for the boundary v_0. We assume without loss of generality that all edge weights are nonzero. We will first consider the normalized Green's function $\mathscr{G}(v_i, v_j) = \mathscr{G}(i, j) = \mathscr{G}(j, i)$ which satisfies, for $x \neq y$,

$$\frac{w_{x-1,x}}{\sqrt{d_x}}\left(\frac{\mathscr{G}(x, y)}{\sqrt{d_x}} - \frac{\mathscr{G}(x-1, y)}{\sqrt{d_{x-1}}}\right) = \frac{w_{x,x+1}}{\sqrt{d_x}}\left(\frac{\mathscr{G}(x+1, y)}{\sqrt{d_{x+1}}} - \frac{\mathscr{G}(x, y)}{\sqrt{d_x}}\right). \tag{14}$$

This implies that for $x < y$,

$$\frac{\mathcal{G}(x, y)}{\sqrt{d_y}} = \frac{\mathcal{G}(x, x)}{\sqrt{d_x}}.$$

Since

$$\frac{w_{x-1, x}}{\sqrt{d_x}} \left(\frac{\mathcal{G}(x, x)}{\sqrt{d_x}} - \frac{\mathcal{G}(x-1, x)}{\sqrt{d_{x-1}}} \right) = 1,$$

we have

$$w_{x-1, x} \left(\frac{\mathcal{G}(x, x)}{d_x} - \frac{\mathcal{G}(x-1, x)}{d_{x-1}} \right) = 1$$

and

$$\frac{\mathcal{G}(x, x)}{d_x} = \frac{1}{w_{x-1, x}} + \frac{1}{w_{x-2, x-1}} + \cdots + \frac{1}{w_{0, 1}}.$$

We can then derive for $G(y, x) = (\sqrt{d_x}/\sqrt{d_y})\ \mathcal{G}(y, x)$ and $G(x, y) = (\sqrt{d_y}/\sqrt{d_x})\ \mathcal{G}(y, x)$

6.2. *The Boundary Has Two Endpoints*

In this subsection, we consider the Green's function G with Dirichlet boundary condition for the boundary $\{v_0, v_{m+1}\}$. From (14), we have, for $x < y$,

$$\begin{aligned}
\mathcal{G}(x, y) &= c_x \sqrt{d_y} \left(\frac{1}{w_{y, y+1}} + \cdots + \frac{1}{w_{m, m+1}} \right) \\
&= c \sqrt{d_x d_y} \left(\frac{1}{w_{y, y+1}} + \cdots + \frac{1}{w_{m, m+1}} \right) \\
&\quad \times \left(\frac{1}{w_{x-1, x}} + \frac{1}{w_{x-2, x-1}} + \cdots + \frac{1}{w_{0, 1}} \right)
\end{aligned}$$

for some constant c. We can then compute c as follows (by extending the above expression to $x = y$):

$$\begin{aligned}
1 &= \mathcal{L}\mathcal{G}(x, x) \\
&= \frac{w_{x-1, x}}{\sqrt{d_x}} \left(\frac{\mathcal{G}(x, x)}{\sqrt{d_x}} - \frac{\mathcal{G}(x-1, x)}{\sqrt{d_{x-1}}} \right) - \frac{w_{x, x+1}}{\sqrt{d_x}} \left(\frac{\mathcal{G}(x+1, x)}{\sqrt{d_{x+1}}} - \frac{\mathcal{G}(x, x)}{\sqrt{d_x}} \right) \\
&= c \sum_y \frac{1}{w_{y-1, y}}.
\end{aligned}$$

Therefore we have

$$c=\left(\sum_{y}\frac{1}{w_{y-1,\,y}}\right)^{-1}$$

and

$$\mathcal{G}(x,\,y)=\frac{\sqrt{d_x d_y}}{\sum_{y}\frac{1}{w_{y-1,\,y}}}\left(\frac{1}{w_{y,\,y+1}}+\cdots+\frac{1}{w_{m,\,m+1}}\right)$$
$$\times\left(\frac{1}{w_{x-1,\,x}}+\frac{1}{w_{x-2,\,x-1}}+\cdots+\frac{1}{w_{0,\,1}}\right)$$

for all $x \leqslant y$.

7. GREEN'S FUNCTION WITH NO BOUNDARY

In the remainder of the paper, we consider the case of Green's functions with no boundary. This case is slightly more difficult than the case with nonempty boundary and Dirichlet boundary conditions. The Laplace operator Δ or the normalized Laplacian $\mathcal{L}$ as defined in Section 2.1 has a zero eigenvalue. Again, we consider a connected finite graph Γ so there is exactly one zero eigenvalue (see [6]). The Green's function G is a matrix with its entries indexed by vertices x and y, defined by

$$G\Delta(x,\,y)=I(x,\,y)-\frac{d_y}{vol},$$

where vol is the sum of all degrees in Γ. Equivalently, the normalized Green's function $\mathcal{G}=T^{-1/2}GT^{1/2}$ satisfies

$$\mathcal{G}\mathcal{L}=\mathcal{L}\mathcal{G}=I-P_0=I-\phi_0^*\phi_0, \tag{15}$$

where P_0 is the projection into the eigenfunction ϕ_0 associated with eigenvalue 0. Here ϕ_0 is taken to be an $n\times 1$ array and the kth entry is $\sqrt{d_k/vol}$. Furthermore, we require that

$$\mathcal{G}P_0=0$$

so that $\mathcal{G}$ is uniquely defined. Let the eigenvalues of $\mathcal{L}$ be denoted by $0=\lambda_0<\lambda_1\leqslant\cdots\leqslant\lambda_{n-1}$ where n is the number of vertices in Γ. It is not hard to see that

$$\mathcal{G} = \sum_{i>0} \frac{1}{\lambda_i} \phi_i^* \phi_i \tag{16}$$

$$= \int_0^\infty (\mathcal{H}_t - P_0)\, dt. \tag{17}$$

To illustrate the usage of Green's functions, we consider the problem of determining the hitting time $Q(x, y)$ from x to y, the expected number of steps for a reversible Markov chain before state y is reached, when started from state x. It is known [1] that the hitting time $Q(x, y)$ satisfies

$$\Delta Q(x, y) = \begin{cases} 1 & \text{if } \quad x \neq y, \\ 1 - \dfrac{vol}{d_x} & \text{if } \quad x = y. \end{cases}$$

Let J denote the all 1's matrix. Then

$$\Delta Q = J - vol\ T^{-1}. \tag{18}$$

We will show the following relation between the hitting time and the Green's function:

THEOREM 8. *The hitting time $Q(x, y)$ satisfies*

$$Q(x, y) = \frac{vol}{d_y}\, G(y, y) - \frac{vol}{d_x}\, G(x, y).$$

Proof. The equation in (18) is equivalent to:

$$\mathcal{L} T^{1/2} Q T^{1/2} = T^{1/2} (J - vol\, T^{-1})\, T^{1/2}$$
$$= vol(\phi_0^* \phi_0 - I).$$

We multiply both sides by $\mathcal{G}$ from the left and we get

$$\mathcal{G} \mathcal{L} T^{1/2} Q T^{1/2} = vol\, \mathcal{G}(\phi_0^* \phi_0 - I)$$
$$= -vol\, \mathcal{G}$$

which implies, by Eq. (15),

$$(I - \phi_0^* \phi_0)\, T^{1/2} Q T^{1/2} = -vol\, \mathcal{G}. \tag{19}$$

By checking the (x, x)-entry of the above equation of matrices and using the fact that $Q(x, x) = 0$, we have

$$(\phi_0^* \phi_0 T^{1/2} Q T^{1/2})(x, x) = \frac{1}{vol} \sum_z d_x d_z Q(z, x)$$

$$= vol\, \mathcal{G}(x, x). \tag{20}$$

By checking the (x, y)-entry of (19), we get

$$\sqrt{d_x d_y}\, Q(x, y) - \frac{1}{vol} \sum_z \sqrt{d_x d_y}\, d_z Q(z, y) = -vol\, \mathcal{G}(x, y). \tag{21}$$

By combining (20) and (21), we have

$$\sqrt{d_x d_y}\, Q(x, y) - \sqrt{\frac{d_x}{d_y}}\, vol\, \mathcal{G}(y, y) = -vol\, \mathcal{G}(x, y). \tag{22}$$

Equivalently, we have

$$\sqrt{d_x d_y}\, Q(x, y) - \sqrt{\frac{d_x}{d_y}}\, vol\, G(y, y) = -vol\, G(x, y) \sqrt{\frac{d_x}{d_x}} \tag{23}$$

as desired. ▮

Next we evaluate the Green's function for a weighted path with no boundary.

THEOREM 9. *Let the vertex set of a path P_n be $\{1, 2, ..., n\}$ and edge weights $w_{x, x+1}$ for $x = 1, ..., n-1$. The normalized Green's function $\mathcal{G}(x, y)$, $x \leqslant y$, for P_n satisfies*

$$\begin{aligned} \mathcal{G}(x, y) &= \mathcal{G}(y, x) \\ &= \frac{\sqrt{d_x d_y}}{vol^2} \left(\sum_{z<x} \frac{(d_1 + \cdots + d_z)^2}{w_{z, z+1}} + \sum_{y \leqslant z} \frac{(d_{z+1} + \cdots + d_n)^2}{w_{z, z+1}} \right. \\ &\quad \left. - \sum_{x \leqslant z < y} \frac{(d_1 + \cdots + d_z)(d_{z+1} + \cdots + d_n)}{w_{z, z+1}} \right) \end{aligned} \tag{24}$$

for $x < y$. The Green's function $G(x, y)$ itself is given by $G(x, y) = \mathcal{G}(x, y) \sqrt{d_y / d_x}$.

Proof. We start from the definition in (15). For $x \neq y$, we have

$$\frac{w_{x-1,x}}{\sqrt{d_x}}\left(\frac{\mathcal{G}(x,y)}{\sqrt{d_x}}-\frac{\mathcal{G}(x-1,y)}{\sqrt{d_{x-1}}}\right)$$
$$=\frac{w_{x,x+1}}{\sqrt{d_x}}\left(\frac{\mathcal{G}(x+1,y)}{\sqrt{d_{x+1}}}-\frac{\mathcal{G}(x,y)}{\sqrt{d_x}}\right)-\frac{\sqrt{d_x d_y}}{vol}. \tag{25}$$

This implies that for $x<y$,

$$\frac{\mathcal{G}(x,y)}{\sqrt{d_x}}-\frac{\mathcal{G}(x-1,y)}{\sqrt{d_{x-1}}}=\frac{\sqrt{d_y}(d_{x-1}+\cdots+d_1)}{vol\, w_{x-1,x}},$$
$$\frac{\mathcal{G}(x,y+1)}{\sqrt{d_{y+1}}}-\frac{\mathcal{G}(x,y)}{\sqrt{d_y}}=-\frac{\sqrt{d_x}(d_{y+1}+\cdots+d_n)}{vol\, w_{y,y+1}}.$$

By telescoping and summing equations of the above types, it leads to the solution in (24). An alternative proof is to directly check that (24) satisfies (25). ∎

EXAMPLE 2. We consider a path P_3 with vertices 1, 2, 3 and edge weights $w_{j,j+1}$. Its Green's function satisfies

$$\mathcal{G}(1,1)=\frac{d_1}{vol^2}\left(\frac{(d_2+d_3)^2}{w_{1,2}}+\frac{d_3^2}{w_{2,3}}\right)$$
$$\mathcal{G}(1,2)=\frac{\sqrt{d_1 d_2}}{vol^2}\left(-\frac{d_1(d_2+d_3)}{w_{1,2}}+\frac{d_3^2}{w_{2,3}}\right)$$
$$\mathcal{G}(1,3)=\frac{\sqrt{d_1 d_3}}{vol^2}\left(-\frac{d_1(d_2+d_3)}{w_{1,2}}-\frac{(d_1+d_2)\,d_3}{w_{2,3}}\right)$$
$$\mathcal{G}(2,2)=\frac{d_2}{vol^2}\left(\frac{d_1^2}{w_{1,2}}+\frac{d_3^2}{w_{2,3}}\right).$$

EXAMPLE 3. We consider a path P_n with edge weights $w_{j,j+1}=1$ for $j=1, ..., n-1$ and $w_{1,1}=w_{n,n}=1$. Its Green's function satisfies

$$G(x,y)=\mathcal{G}(x,y)$$
$$=\frac{1}{n^2}\left(\sum_{z<x} z^2+\sum_{z\leqslant n-y} z^2-\sum_{x\leqslant z<y} z(n-z)\right)$$
$$=\frac{1}{n^2}\left(\frac{(y-1)\,y(2y-1)}{6}+\frac{(n-y)(n-y+1)(2n-2y+1)}{6}\right.$$
$$\left.-\frac{n(x+y-1)(y-x)}{2}\right).$$

EXAMPLE 4. We consider the Green's function for an n-cube Q_n with 2^n vertices represented by binary n-tuples. Two vertices are adjacent if the corresponding n-tuples differ at exactly one coordinate. Clearly, Q_n is distance regular. The projected weighted path has edge weights $w_{j,\,j+1} = \binom{n}{j}$, for $j = 0, ..., n-1$. By using the Green's function $\mathcal{G}$ of the weighted path, we can derive the Green's function $\tilde{G}(x, y)$ for two vertices at distance k in Q_n, for $k > 0$.

$$\tilde{G}(x, y) = \frac{\mathcal{G}(0, k)}{\binom{n}{k}}$$

$$= 2^{-2n}\left(-\sum_{j<k} \frac{\left(\binom{n}{0} + \cdots + \binom{n}{j}\right)\left(\binom{n}{j+1} + \cdots + \binom{n}{n}\right)}{\binom{n-1}{j}} + \sum_{k \leqslant j} \frac{\left(\binom{n}{j+1} + \cdots + \binom{n}{n}\right)^2}{\binom{n-1}{j}} \right)$$

So, by Theorem 8, the hitting time between two vertices of distance j in Q_n is

$$2^n(\tilde{G}(y, y) - \tilde{G}(x, y)) = 2^{-n}\left(\sum_{j<k} \frac{\left(\binom{n}{j+1} + \cdots + \binom{n}{n}\right)^2}{\binom{n-1}{j}} + \sum_{j<k} \frac{\left(\binom{n}{0} + \cdots + \binom{n}{j}\right)\left(\binom{n}{j+1} + \cdots + \binom{n}{n}\right)}{\binom{n-1}{j}} \right)$$

$$= \sum_{j<k} \frac{\binom{n}{j+1} + \cdots + \binom{n}{n}}{\binom{n-1}{j}}.$$

This gives an alternative proof for the expected hitting time for the n-cube, which was previously examined by Pomerance and Winkler [22].

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