Spectral Graph Theory and Discrete Poisson Equation

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In this report, we summarize the main definitions of spectral graph theory and focus in particular on their use in solving a discrete version of the Poisson equation that arises in applicative problems.

1 Graph Laplacian

Spectral graph theory provides a bridge between the combinatorial structure of a graph and its geometric properties. While the adjacency matrix describes local connectivity, the Laplacian spectrum governs global processes like diffusion, random walks, and the stability of dynamical systems. In particular, solving the discrete Poisson equation, which arises in problems like electric flow, requires understanding the "harmonics" of the graph, which correspond to the eigenfunctions of the Laplacian.

The references for the report are [1] and [2]. We generally follow the notation from [2], although [1] being the main reference for Section 1 and [2] for Section 2.

1.1 Basic Definitions

Let $\Gamma = (V, E)$ be an undirected weighted graph with weights defined as a function $w : V \times V \to \mathbb{R}; (x, y) \mapsto w_{x,y}$. We consider a graph without parallel edges and possibly with loops. Given $x, y \in V$, we write $x \sim y$ to intend x connected to y and $d_x := \sum_{y \in V} w_{x,y}$. We give the following definitions.

Definition 1. *We call* discrete Laplacian *of the graph* Γ *(or,* random-walk Laplacian*) the following matrix with rows and columns corresponding to vertices*

$$\Delta(x, y) := \begin{cases} 1 - w_{x,x}/d_x, & \text{if } x = y \text{ and } d_x \neq 0; \\ -w_{x,y}/d_x, & \text{if } x \sim y; \\ 0, & \text{otherwise.} \end{cases}$$

Definition 2. *Given the adjacency matrix* A *of* Γ *and* D *the diagonal matrix with* $D(x, x) = d_x$ *for* $x \in V$*, we define the* combinatorial Laplacian *matrix* $L = D - A$.

As said before, we are interested in computing the eigenvalues of the Laplacian as a summary description of the main properties of the graph; the matrix Δ, however, is in general non-symmetric. To exploit spectral properties given by symmetry, we can overcome the problem by defining the *normalized Laplacian*.

Definition 3. *We define* normalized Laplacian *matrix the matrix* $\mathcal{L}$

$$\mathcal{L} := D^{1/2} \Delta D^{-1/2}$$

Remark 1.

- *$\mathcal{L}$ can also be defined as $\mathcal{L} = D^{-1/2} L D^{-1/2}$;*
- *$\mathcal{L}$ is similar to Δ, therefore they have the same eigenvalues;*
- *$\mathcal{L}$ is symmetric, therefore, by spectral theorem, its eigenvalues are real, non-negative and the eigenfunctions can be taken orthonormal.*

Remark 2. *We can interpret the Laplacian Δ as an operator on the functions $f : V \to \mathbb{R}$ by writing f as a vector and defining Δf as a matrix-vector multiplication which leads to the formula*

$$\Delta f(x) = \sum_{y \in V} (f(x) - f(y)) \frac{w_{x,y}}{d_x}, \quad \forall x \in V \tag{1}$$

This interpretation connects the discrete Laplacian with its continuous counterpart.

To study the eigenvalues of $\mathcal{L}$, we can use a variational characterization, summarized in the following.

Proposition 3. *Let $\lambda_0 \leq \lambda_1 \leq \cdots \leq \lambda_{n-1}$ be the eigenvalues of $\mathcal{L}$, then*

(i) $\lambda_0 = 0$*, by taking as eigenfunction $D^{1/2}\mathbf{1}$, where $\mathbf{1}(x) := 1 \ \forall x$;*

(ii) $\lambda_1 = \inf_{g \perp D^{1/2}\mathbf{1}} \frac{\langle g, \mathcal{L} g \rangle}{\langle g, g \rangle} = \inf_{f : \sum_x f(x) d_x = 0} \frac{\sum_{x \sim y} (f(x) - f(y))^2 w_{x,y}}{\sum_x f^2(x) d_x}$*;*

(iii) $\lambda_{n-1} = \sup_f \frac{\sum_{x \sim y} (f(x) - f(y))^2 w_{x,y}}{\sum_x f^2(x) d_x}$.

Remark 4. *As said before, the eigenvalues can be seen as summary of graph properties by the following interpretation:*

- *The multiplicity of λ_0 is the number of connected components of the graph, since, for each connected component, we can take as eigenfunction $D^{1/2}\mathbf{1}$ on one connected component and 0 everywhere else.*
- *$\lambda_{n-1} \leq 2$ and $\lambda_{n-1} = 2$ if and only if the graph is bipartite: in this case we can take an eigenfunction equal to $D^{1/2}\mathbf{1}$ on a set of the partition and $-D^{1/2}\mathbf{1}$ on the other;*
- *The quantity $\sum_{x,y}(f(x) - f(y))^2 w_{x,y}$ is called* Dirichlet energy *of f and it is the discrete counterpart of the Dirichlet energy $\int_\Omega |\nabla u(x)| dx$ for $u : \Omega \subseteq \mathbb{R}^d \to \mathbb{R}$. As for the continuous version, the Dirichlet energy on the graph measures how much the function f "oscillates" on its domain.*

  λ_1, also called spectral gap*, quantifies the "expansivity" of the graph: a small λ_1 implies the existence of a sparse cut. In the context of the Dirichlet energy, if λ_1 is small, there exists a non-constant function f with very low energy, meaning the graph has a "bottleneck" that allows f to stay nearly constant on large clusters while changing slowly across the few connecting edges.*

An important property of λ_1 related to the "expansivity" feature is Cheeger inequality, that we state for the sake of completeness, but not elaborate further.

Proposition 5. *It holds the* Cheeger inequality

$$2h(G) \leq \lambda_1 \leq \frac{h^2(G)}{2 \max_x d_x}$$

where $h(G) = \min \left\{ \frac{|\delta A|}{|A|} : A \subseteq V, 0 < |A| \leq \frac{1}{2}|V| \right\}$ *is the* Cheeger constant *and* $\delta A := \{(x, y) \in E : x \in A, y \in V \setminus A\}$

2 Discrete Poisson Equation

We want now to use the definitions from the previous section to make sense of the equation

$$\Delta f(x) = g(x) \tag{2}$$

for f and g functions defined on V.

The equation is an interesting object in itself, but its definition gains motivation from some problems of applicative interest. A typical example are Electrical Networks: if the graph is viewed as a resistive circuit where $w_{x,y}$ represents the conductance between nodes, $f(x)$ represents the electric potential. The equation $\Delta f = g$ is then a statement of Kirchhoff's Current Law, where g represents the current injected into the network at each node.

2.1 Problem

To make sense of equation (2), we consider $S \subseteq V$ and define the boundary of S as $\partial S := \{y \notin S : w_{x,y} \neq 0 \text{ for some } x \in S\}$. We will assume S connected and $\partial S \neq \emptyset$ such that Δ_S, the Laplacian corresponding to the subgraph with vertices in S is non-singular.

Definition 4. *Given $g : S \to \mathbb{R}$ and $\sigma : \partial S \to \mathbb{R}$, we say $f : S \cup \partial S \to \mathbb{R}$ solves the* discrete Poisson equation *on S if*

$$\begin{cases} \Delta_S f(x) = g(x), & \text{for } x \in S; \\ f(x) = \sigma(x), & \text{for } x \in \partial S. \end{cases} \tag{3}$$

where Δ_S is obtained from Δ keeping only rows and columns corresponding to S.

To solve the discrete Poisson equation, one can proceed analogously to the continuous case by defining a discrete counterpart of Green's function.

Definition 5. *We define* discrete Green's function *for Δ_S as the inverse of the Laplace operator Δ_S, namely the linear operator G_S such that*

$$G_S \Delta_S = I$$

where I is the identity operator.

We define the normalized Green's function *as*

$$\mathcal{G}_S = D^{1/2} G_S D^{-1/2}$$

Remark 6. *The assumptions of connectivity on S which make Δ_S non-singular are required to give the previous definitions of G_S and $\mathcal{G}_S$.*

The Green's function can be written explicitly in analogy with the continuous case as solution of a discrete heat equation.

Definition 6. *Given $t \geq 0$ and $S \subseteq V$, we define* discrete heat kernel *of S*

$$\mathcal{H}_t(x, y) = \sum_{i=1}^{s} e^{-\lambda_i t} \varphi_i(x) \varphi_i(y)$$

where λ_i, φ_i are respectively the i-th eigenvalue and the i-th eigenfunction of $\mathcal{L}_S$, the matrix obtained from $\mathcal{L}$ by keeping only the rows and columns corresponding to vertices in S.

Remark 7. *By definition $\mathcal{H}_t$ intended as linear operator satisfies the following heat equation,*

$$\begin{cases} \frac{d}{dt} \mathcal{H}_t f = -\mathcal{L}_S(\mathcal{H}_t f), & \text{on } S; \\ f = \sigma, & \text{on } \partial S. \end{cases}$$

The explicit formulation of the Green's function follows from the spectral decomposition of $\mathcal{L}_S$.

Lemma 8. *It holds*

$$\mathcal{G}_S(x, y) = \sum_i \frac{1}{\lambda_i} \varphi_i(x) \varphi_i(y)$$

following the definition $\mathcal{G}_S \mathcal{L}_S = I = \mathcal{L}_S \mathcal{G}_S$.

Proposition 9. *Since* $\int_0^\infty e^{-t\lambda}dt = 1/\lambda_i$,

$$\mathcal{G}_S = \int_0^\infty \mathcal{H}_t dt$$

Renormalizing, we obtain

$$G_S(x,y) = \int_0^\infty d_x^{1/2}\mathcal{H}_t(x,y)d_y^{-1/2}dt = \sum_i \frac{1}{\lambda_i} d_x^{1/2}\varphi_i(x)\varphi_i(y)d_y^{-1/2}, \qquad \text{for } x,y \in S.$$

To find a solution of the discrete Poisson equation, we proceed in analogy to what is done to find a solution of the Poisson PDE in the continuous case by first defining a solution for the homogeneous equation with boundary conditions and then combining it with a solution for the non-homogeneous case with null boundary conditions.

Proposition 10. $f : S \cup \partial S \to \mathbb{R}$ *solution of* (3) *with* $g = 0$ *can be written as*

$$f(z) = \sum_i \left(\frac{1}{\lambda_i} \sum_{x \in S : x \sim y \in \partial S} \sqrt{d_x}\varphi_i(x)\sigma(y) \right) d_z^{-1/2}\varphi_i, \quad \forall z \in S$$

where φ_i *are the eigenfunctions of* $\mathcal{L}_S$.

Sketch of the proof: The idea of the proof is to define $\tilde{f}(x) = D^{1/2}f(x)$ and deduce from $\mathcal{L}_S\tilde{f} = 0$ that $\tilde{f} = \sum_i \langle \varphi_i, \tilde{f}\rangle\varphi_i$. The coefficients $\langle \varphi_i, \tilde{f}\rangle$ then follow explicit computations that exploit the boundary condition. □

Proposition 11. $f : S \cup \partial S \to \mathbb{R}$ *solution of* (3) *with* $\sigma = 0$ *can be written as*

$$f = G_S g$$

where G_S *is the Green's function for* Δ_S.

Proposition 12. *A general solution* f *for* (3) *can be written as* $f = f_1 + f_2$ *where* f_1 *is a solution of* $\Delta f_1(x) = 0$ *with boundary condition* $f_1 \equiv \sigma$ *on* ∂S *and* f_2 *is a solution of* $\Delta f_2(x) = g(x)$ *with boundary condition* $f_2 \equiv 0$ *on* ∂S.

2.2 Application: Expected Hitting Times

A classical application of Poisson equation is to theory of Markov chains. Let us consider a Markov Chain, and S an (irreducible) set of states. We can represent the Markov chain process as a random walk on a graph where transition probabilities are proportional to weights of the graph. Since S is irreducible, the corresponding subgraph is connected and thus the Green's function well-defined. We call *expected hitting time* $h(x)$ the average number of steps of a random walk starting at $x \in S$ takes to reach the boundary ∂S, that we assume nonempty. Then the following result holds.

Proposition 13. *The hitting time function* $h : S \cup \partial S \to \mathbb{R}$ *is the unique solution to the discrete Poisson equation:*

$$\begin{cases} \Delta_S h(x) = 1, & \text{for } x \in S; \\ h(x) = 0, & \text{for } x \in \partial S. \end{cases} \tag{4}$$

References

[1] F. R. K. Chung. *Spectral Graph Theory.* American Mathematical Society, 1997.

[2] Fan Chung and S.-T. Yau. "Discrete Green's Functions". In: *Journal of Combinatorial Theory, Series A* 91.1 (2000), pp. 191–214.