Spectral Graph Theory and Discrete Poisson Equation

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Presentation for the exam of *Graph Theory*

Goal

Summarize principal properties of a graph into a simple list of invariants.

Spectral Graph Theory

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$\rightarrow$ Write graph information in a **matrix**;

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Adjacency matrix $\rightsquigarrow$ **Laplacian matrix**

Graph Laplacian

Let $G = (V, E)$ be an **undirected** graph; $d_x := \sum_{y \in V} w_{x,y}$ degree of $x \in V$.

Graph Laplacian

We define **graph Laplacian** the matrix

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

$\rightarrow$ **Idea:** summarize graph information in Laplacian eigenvalues.

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→ **Idea:** summarize graph information in Laplacian eigenvalues.

→ **Problem:** Δ is in general non-symmetric. We can consider the **normalized Laplacian**

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

where D is the diagonal matrix with $D(x,x) = d_x$.

Graph Laplacian

Let $G = (V, E)$ be an **undirected** graph; $d_x := \sum_{y \in V} w_{x,y}$ degree of $x \in V$.

Graph Laplacian [Fan Chung, *Spectral Graph Theory*]

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Note: A different definition is the **combinatorial Laplacian** $L = D - A$ with A adjacency matrix and $\mathcal{L} = D^{-1/2} L D^{-1/2}$.

Motivating Example

Matrix-tree Theorem

The number of spanning trees in a graph G is

$$\frac{\prod_i \lambda_i \prod_{x \in S} d_x}{\sum_{x \in S} d_x}$$

where S is any maximum proper subset of the vertex set and λ_i are the eigenvalues of L restricted to S.

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Spectral Convergence of Markov Chains

Let p_t be the distribution after t steps of a lazy random walk on a connected graph G and $\pi(x) = \frac{d_x}{\sum_{y \in V} d_y}$ the stationary distribution. Then,

$$\|p_t - \pi\|_2 \leq \max_{i \geq 1} \left\{ \left| 1 - \frac{\lambda_i}{2} \right| \right\}^t \sqrt{\frac{\max_x d_x}{\min_y d_y}}$$

Laplacian

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Why Laplacian?

Let $f : V \to \mathbb{R}$. We can interpret f as a vector $(f(x))_{x\in V}$ and write $\Delta \cdot f$, thus

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

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Intuition

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3-vertices path with weight 1 for each edge:

$$f : V \to \mathbb{R} \rightsquigarrow \Delta f(x) = \frac{2f(x) - f(x-1) - f(x+1)}{2}$$

$$f : \Omega \subseteq \mathbb{R} \to \mathbb{R} \rightsquigarrow \Delta f(x) = f''(x)$$

Smallest Eigenvalue

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

λ_0

$\lambda_0 \leq \lambda_1 \leq \cdots \leq \lambda_{n-1}$ eigenvalues of Δ, it holds

- $\lambda_0 = 0$ by taking $f \equiv 1$ on a connected component and 0 everywhere else.

$\rightarrow$ Its multeplicity represents the connected components of G.

Second Smallest Eigenvalue

Variational Characterization of λ_1

$0 = \lambda_0 \leq \lambda_1 \leq \cdots \leq \lambda_{n-1}$ eigenvalues of $\mathcal{L}$, it holds

$$\lambda_1 = \inf_{f : \sum_x f(x) d_x = 0} \frac{\overbrace{\sum_{x \sim y} (f(x) - f(y))^2 w_{xy}}^{\text{Dirichlet energy}}}{\sum_x f^2(x) d_x}$$

$\rightarrow$ Measures “connectivity” of the graph.

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$\rightarrow$ Measures "connectivity" of the graph. **Formal intuition**: *Cheeger Inequality*

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

where $h(G) = \min \left\{ \frac{|\delta A|}{|A|} : A \subseteq V, 0 < |A| \leq \frac{1}{2}|V| \right\}$

and $\delta A := \{(x, y) \in E : x \in A, y \in V \setminus A\}$

Greatest Eigenvalue

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

λ_{n-1}

$0 = \lambda_0 \leq \lambda_1 \leq \cdots \leq \lambda_{n-1}$ eigenvalues of Δ, it holds

- $\lambda_{n-1} \leq 2$;
- $\lambda_{n-1} = 2 \iff$ the graph is bipartite.

$\rightarrow$ By taking $f \equiv 1$ on a set of the partition and $f \equiv -1$ to the other set.

Example: Path Graph P_3

Setting: Path graph P_3 $>>$

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Laplacian

$$\Delta = \begin{pmatrix} 1 & -1 & 0 \\ -1/2 & 1 & -1/2 \\ 0 & -1 & 1 \end{pmatrix} \quad \rightsquigarrow \quad \mathcal{L} = D^{1/2} \Delta D^{-1/2} = \begin{pmatrix} 1 & -1/\sqrt{2} & 0 \\ -1/\sqrt{2} & 1 & -1/\sqrt{2} \\ 0 & -1/\sqrt{2} & 1 \end{pmatrix}$$

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Eigenvalues:

- $\lambda_0 = 0$ (one connected component);
- $\lambda_1 = 1$ (graph “well-connected”);
- $\lambda_2 = 2$ (graph is bipartite).

Example: Triangle T_3

Setting: Triangle graph T_3 >>

Normalized Laplacian:

$$\mathcal{L} = \begin{pmatrix} 1 & -\frac{1}{2} & -\frac{1}{2} \\ -\frac{1}{2} & 1 & -\frac{1}{2} \\ -\frac{1}{2} & -\frac{1}{2} & 1 \end{pmatrix}.$$

Eigenvalues:

- $\lambda_0 = 0$ (one connected component);
- $\lambda_1 = 3/2$ (graph “fully connected”);
- $\lambda_2 = 3/2 < 2$ (graph not bipartite).

Example: The 3-Star S_3

Setting: Star graph S_3 >>

Normalized Laplacian:

$$\mathcal{L} = \begin{pmatrix} 1 & -\frac{1}{\sqrt{3}} & -\frac{1}{\sqrt{3}} & -\frac{1}{\sqrt{3}} \\ -\frac{1}{\sqrt{3}} & 1 & 0 & 0 \\ -\frac{1}{\sqrt{3}} & 0 & 1 & 0 \\ -\frac{1}{\sqrt{3}} & 0 & 0 & 1 \end{pmatrix}.$$

Eigenvalues:

- $\lambda_0 = 0$ (one connected component);
- $\lambda_1 = \lambda_2 = 1$ (graph "well-connected", symmetry);
- $\lambda_3 = 2$ (graph is bipartite).

Discrete Poisson Equation

Discrete Poisson Equation

$S \subseteq V$, $\partial S := \{y \notin S : w_{x,y} \neq 0$ for some $x \in S\}$

Equation [Chung, Yau, *Discrete Green's Functions*]

For $f : S \cup \partial S \to \mathbb{R}$, $g : S \to \mathbb{R}$ and $\sigma : \partial S \to \mathbb{R}$

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

Motivating Example

Electric Networks

Let $G = (V, E)$ represent an **electric network**, the discrete Poisson equation is used to describe **diffusion**.

- g: external current source on the network;
- f: potential at the nodes;
- σ: fixed potential it in the boundary vertices.

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

Solving Discrete Poisson Equation

Solution Strategy

As for continuous PDEs,

$\rightarrow$ Find $f^{(1)}$ solution of

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→ Define the solutions of the discrete Poisson equation as $f = f^{(1)} + f^{(2)}$

Solution of $\Delta f^{(1)} = 0$

Solution form

$f^{(1)}$ solution of

$$\begin{cases} \Delta_S f(x) = 0, & \text{for } x \in S; \\ f(x) = \sigma(x), & \text{for } x \in \partial S. \end{cases}$$

have the form

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

where λ_i eigenvalues and φ_i eigenfunctions of Δ_S.

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Proof idea

→ We consider $\tilde{f}^{(1)}(x) = D^{1/2} f^{(1)}(x)$ satisfying $\mathcal{L}_S \tilde{f}^{(1)}(x) = 0$ on S.

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- → We consider $\tilde{f}^{(1)}(x) = D^{1/2} f^{(1)}(x)$ satisfying $\mathcal{L}_S \tilde{f}^{(1)}(x) = 0$ on S.
- → We can write $\tilde{f}^{(1)} = \sum_i \langle \varphi_i, \tilde{f}^{(1)} \rangle \varphi_i$.

Solution of $\Delta f^{(1)} = 0$

Solution form

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

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- → We can write $\tilde{f}^{(1)} = \sum_i \langle \varphi_i, \tilde{f}^{(1)} \rangle \varphi_i$.
- → Explicitly compute $\langle \varphi_i, \tilde{f}^{(1)} \rangle$ using the boundary condition σ.

Particular solution of $\Delta f^{(2)} = g$

Discrete Green's Function

If $\partial S \neq \emptyset$ and S is connected, we define the **Discrete Green's Function** G_S as

$$G_S \Delta_S = I$$

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We have

$$G_S(x,y) = \sum_i \frac{1}{\lambda_i} d_x^{1/2} \varphi_i(x) \varphi_i(y) d_y^{-1/2}, \quad \text{for } x, y \in S.$$

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Solution form

We can take as solution of $\Delta_S f^{(2)} = g$ with boundary condition $f^{(2)} = 0$ on ∂S the function

$$f^{(2)} = G_S g$$

Solution of Discrete Poisson Equation

Solution Form

Solution of the Discrete Poisson Equation

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

are of the form $f = f^{(1)} + f^{(2)}$ with $f^{(1)}$ and $f^{(2)}$ computed as in the previous slides.

Application: Hitting Probability

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Discrete Poisson Equation: $f_{x,y}(z)$ is the solution of

$$\begin{cases} \Delta_S f_{x,y}(z) = 0, & z \in S \\ f_{x,y}(z) = \sigma(z), & z \in \partial S \end{cases}$$

Application: Hitting Probability

Setting: P_3 path graph.

Solution: We can compute explicitly $\Delta f_{1,3}(2) = 0$ with boundary conditions $\sigma(1) = 1, \sigma(3) = 0$.

$$\frac{2f_{1,3}(2) - f_{1,3}(1) - f_{1,3}(3)}{2} = 0 \implies \frac{2f_{1,3}(2) - 1 - 0}{2} = 0 \implies f_{1,3}(2) = \frac{1}{2}$$

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- the spectrum of a graph is defined as the spectrum of the **discrete Laplacian** Δ on the graph;
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- computation of the spectrum of the graph can be used to define the solutions of the equation; these solution come up in applications.

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Thank you for your attention!