A Final Remark on Discrete Nodal Domain Theorem.

Discrete Nodal Domain Theorems actually holds for a large class of discrete Laplacian-type operators. Recall for the graph Laplacian: $\forall f: V \to \mathbb{R}$, $\Delta f: V \to \mathbb{R}$ is given by

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

Denote all vertices of V as $x_1, \cdots, x_{|V|}$. There exists a $|V| \times |V|$ Laplacian matrix

$$\begin{array}{c} \\ x_1 \\ \vdots \\ x_{|V|} \end{array} \begin{array}{c} \begin{array}{ccc} x_1 & \cdots & x_{|V|} \end{array} \\ \begin{pmatrix} & & \\ & \Delta & \\ & & \end{pmatrix} \end{array} \begin{pmatrix} f(x_1) \\ \vdots \\ f(x_{|V|}) \end{pmatrix} = \begin{pmatrix} \Delta f(x_1) \\ \vdots \\ \Delta f(x_{|V|}) \end{pmatrix}.$$

It is direct to check

$$\Delta_{x_i x_j} = \begin{cases} -1, & \text{if } x_i = x_j \\ \frac{1}{d_{x_i}}, & \text{if } x_i \sim x_j \\ 0, & \text{otherwise}. \end{cases}$$

That is, in matrix form, we have

$$-\Delta = D^{-1}(D - A) = I - D^{-1}A$$

where $D = \begin{pmatrix} d_{x_1} & & 0 \\ & \ddots & \\ 0 & & d_{x_{|V|}} \end{pmatrix}$, is the diagonal degree matrix.

$$A_{x_i x_j} = \begin{cases} 1 & \text{if } x_i \sim x_j \\ 0 & \text{if } x_i \not\sim x_j \end{cases}$$ is the adjacency matrix.

In the previous discussions, we prove various discrete nodal domain theorems for the eigenfunctions of the matrix $-\Delta = D^{-1}(D - A)$ eigenvectors

~~$+\Delta = D^{-1}A - I = D^{-1}(A - D)$~~.

There is a symmetric matrix associated to $-\Delta$, which is known as Chung's normalized Laplacian,

$$\mathcal{L} := D^{-\frac{1}{2}}(-\Delta)D^{-\frac{1}{2}} = D^{\frac{1}{2}}(I - D^{-1}A)D^{-\frac{1}{2}}$$

$$= I - D^{-\frac{1}{2}} A D^{-\frac{1}{2}}.$$

Indeed, $$\mathcal{L}_{x_i x_j} = \begin{cases} 1, & \text{if } x_i = x_j \\ -\dfrac{1}{\sqrt{d_{x_i} d_{x_j}}}, & \text{if } x_i \sim x_j \\ 0. & \text{otherwise} \end{cases}$$

Obviously, the matrix $\mathcal{L}$ and $(-\Delta)$ share the same eigenvalues.

- f is an eigenvector of $\mathcal{L}$ iff $D^{-\frac{1}{2}} f$ is an eigenvector of $-\Delta$.

(i.e., $\mathcal{L} f = \lambda f \Leftrightarrow D^{\frac{1}{2}}(-\Delta)D^{-\frac{1}{2}} f = \lambda f \Leftrightarrow (-\Delta)(D^{-\frac{1}{2}} f) = \lambda (D^{-\frac{1}{2}} f)$)

Therefore, all nodal domain theorems also holds for $\mathcal{L}$.

In fact, all nodal domain theorems we discussed hold for a "generalized Laplacian" on a graph $G = (V, E)$.

We call a ~~symmetric~~ matrix $M = \begin{array}{c|c} & x_1 \cdots x_{|V|} \\ \hline \begin{matrix} x_1 \\ \vdots \\ x_{|V|} \end{matrix} & \begin{pmatrix} & & \\ & & \\ & & \end{pmatrix} \end{array}$ a <u>generalized Laplacian</u> if

(i) M is symmetric.

(ii) $M_{x_i x_j} < 0$ whenever $x_i \sim x_j$

(iii) $M_{x_i x_j} = 0$ whenever $x_i \neq x_j$ and $x_i \not\sim x_j$.

Notice that, we do not have any restriction on the diagonal entries.

Of course, Chung's Laplacian $\mathcal{L}$ is a generalized Laplacian.

We can freely add diagonal entries to M. In operator

form, this means we can add a potential term freely. Therefore, a generalized Laplacian is also called a discrete Schrödinger operator. Discrete Nodal Domain Theorem (DNDT) holds for any generalized Laplacian. (See [BLS]).

In fact, from the above discussion, we can ~~introduce~~ reformulate the definition of generalized Laplacian as below:

An linear operator $L : \mathbb{R}^{|V|} \to \mathbb{R}^{|V|}$ is called a generalized Laplacian, if.

(i) $\exists$ a vertex measure $\mu : V \to \mathbb{R}_{>0}$ s.t. L is self-adjoint in the sense of: $(Lf, g)_\mu = (f, Lg)_\mu$, where $(f, g)_\mu := \sum_{x \in V} f(x) g(x) \mu(x)$.

(ii) $(\delta_{x_i}, L\delta_{x_j})_\mu < 0$ whenever $x_i \sim x_j$

(iii) $(\delta_{x_i}, L\delta_{x_j})_\mu = 0$ whenever $x_i \neq x_j$ and $x_i \sim x_j$

DNDT holds for any such operator L. (Excercise)

<u>Particular examples</u>:

(1) Weighted graph Laplacian:

$\forall f : V \to \mathbb{R}$, $\Delta f : V \to \mathbb{R}$ is given by

$$\Delta f(x) = \frac{1}{\mu(x)} \sum_{y \in V} w_{xy} (f(y) - f(x))$$

where $\mu : V \to \mathbb{R}_{>0}$ is a vertex measure, and $w_{xy} \in \mathbb{R}_{\geq 0}$, $w_{xy} \neq 0$ whenever $x \sim y$, is a set of edge weights. Then $-\Delta$ is a generalized Laplacian.

(2). Dirichlet Laplacian: Let $G=(V,E)$. (could be infinite)

$\forall\, \Omega \overset{\text{finite}}{\subset} V$, consider

$$\begin{cases} \Delta f(x) + \lambda f(x) = 0, & \forall x \in \Omega \\ f(y) = 0, & \forall y \in V \setminus \Omega \end{cases}$$

where Δ is the Laplacian of G.

Let us denote G^Ω to be the subgraph of G induced on Ω.

Define $\forall\, h: \Omega \to \mathbb{R}$, $\Delta^\Omega h : \Omega \to \mathbb{R}$ by

$$\Delta^\Omega h(x) := \Delta \bar{h}(x), \qquad \forall x \in \Omega.$$

where $\bar{h}: V \to \mathbb{R}$ is given by $\bar{h}(y) = \begin{cases} h(y), & \text{if } y \in \Omega \\ 0, & \text{if } y \in V \setminus \Omega \end{cases}$

Then its not hard to check $-\Delta^\Omega$ is a generalized Laplacian on G^Ω.

(II) Connectedness, bipartiteness, and extremal eigenvalues

In this chapter, we discuss the geometric information hidden in the extremal eigenvalues $0=\lambda_1$, λ_2 and $\lambda_{|V|}$.

Recall that

G is connected iff $\lambda_2 > 0$

G is bipartite iff $\lambda_{|V|} < 2$.

(II.1) Motivations: convergence to equilibrium.

Consider a discrete-time heat equation on a graph $G=(V,E)$.

That is,
$$\begin{cases} f(x,t+1) - f(x,t) = \Delta f(x,t) & t=0,1,2,\cdots \\ & x \in V. \\ f(x,0) = f_0(x). \end{cases}$$

where $f: V\times\{0,1,2,\cdots\} \to \mathbb{R}$, $f_0 : V \to \mathbb{R}$.

A natural question is that, how $f(\cdot,t)$ behaves as $t \to \infty$?

Observe that for any t,

$$f(x,t+1) - f(x,t) = \frac{1}{d_x}\sum_{y:y\sim x}(f(y,t) - f(x,t))$$
$$= \frac{1}{d_x}\sum_{y:y\sim x} f(y,t) - f(x,t)$$

$$\Rightarrow f(x,t+1) = \frac{1}{d_x}\sum_{y:y\sim x} f(y,t) := Pf(x,t).$$

where we introduce a new operator P s.t.

$$Ph(x) := \frac{1}{d_x}\sum_{y:y\sim x} h(y)$$

From $$f(x,t+1) = Pf(x,t), \quad \forall t$$

we obtain iteratively that

$$f(x,t) = Pf(x,t-1) = P^2 f(x,t-2)$$
$$= \cdots = P^t f(x,0) = P^t f_0(x).$$

For any $f: V \to \mathbb{R}$, we define $\|f\| := \sqrt{(f,f)}$.

<u>Theorem 1</u>. Let $G=(V,E)$ be a finite simple, connected graph. For any function $f_0: V \to \mathbb{R}$, set

$$\bar{f}_0(y) = \frac{1}{vol(G)} \sum_{x \in V} f_0(x)\, d_x, \quad \forall y \in V.$$

Then ~~we have~~ the solution of discrete-time heat eq. satisfies:

$$\|f(\cdot,t) - \bar{f}_0\| \le \rho^n \|f_0\|, \qquad (*)$$

where $$\rho = \max\{|1-\lambda_2|, |1-\lambda_{|V|}|\}.$$

Consequently, if the graph G is not bipartite, then

$$\|f(x,t) - \bar{f}_0\| \to 0 \quad \text{as } t \to \infty,$$

that is, $f(x,t)$ converges to a constant function $\bar{f}_0$ as $t \to \infty$.

<u>Proof</u>: We only need to show $(*)$. Choose an orthogonal basis $\{f_k\}_{k=1}^{|V|}$ of eigenfunctions of Δ, Then

$$\lambda_k f_k = -\Delta f_k = (I-P) f_k \Rightarrow \boxed{Pf_k = (1-\lambda_k) f_k}.$$

For any function $f_0: V \to \mathbb{R}$, it can be expanded as

$$f_0 = \sum_{k=1}^{|V|} a_k f_k \,, \quad \text{where } a_k = (f_0, f_k).$$

We calculate

$$\|f_0\|^2 = \sum_{k=1}^{|V|} a_k^2 .$$

and $$Pf_0 = \sum_{k=1}^{|V|} a_k P f_k = \sum_{k=1}^{|V|} a_k (1-\lambda_k) f_k ,$$

and by induction, we have

$$f(\cdot, t) = P^t f_0(\cdot) = \sum_{k=1}^{|V|} a_k (1-\lambda_k)^t f_k(\cdot) .$$

We pay particular attention to a_1 and f_1. Since f_1 is constant, and $(f_1, f_1) = \sum_{x\in V} f_1(x)^2 d_x = 1$, we derive

$$f_1(x) \equiv \frac{1}{\sqrt{Vol(G)}}$$

Therefore $$a_1 = (f_0, f_1) = \sum_{x\in V} f_0(x) f_1(x)\, d_x$$

$$= \frac{1}{\sqrt{Vol(G)}} \sum_{x\in V} f_0(x)\, d_x \cancel{= \bar{f}_0(y), \forall y.}$$

$$\Rightarrow a_1 f_1 = \bar{f}_0 .$$

Hence we have

$$f(\cdot,t) - \bar{f}_0 = \sum_{k=1}^{|V|} a_k (1-\lambda_k)^t f_k - a_1 f_1$$

$$= \sum_{k=2}^{|V|} (1-\lambda_k)^t a_k f_k .$$

That is, $$\|f(\cdot,t) - \bar{f}_0\|^2 = \sum_{k=2}^{|V|} (1-\lambda_k)^{2t} a_k^2$$

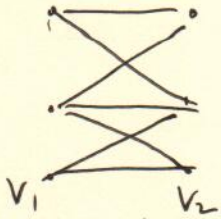
$$\le \max_{2\le k\le |V|} |1-\lambda_k|^{2t} \sum_{k=2}^{|V|} a_k^2$$

$$\le \max_{2\le k\le |V|} |1-\lambda_k|^{2t} \|f_0\|^2$$

Since $1-\lambda_{|V|} \le 1-\lambda_k \le 1-\lambda_2$, $\forall\ 2\le k\le |V|$, we arrive at.

$$\|f(\cdot,t) - \bar{f}_0\|^2 \le \max\{|1-\lambda_2|^{2t}, |1-\lambda_{|V|}|^{2t}\} \|f_0\|^2 . \quad \square$$

<u>Remark</u>: If we start with $f_0 := \delta_x$, $x \in V$. Then the function $f(x, t)$ is just the ~~distribu~~ distribution function of a random walker starting from $x \in V$ at the t-th step.



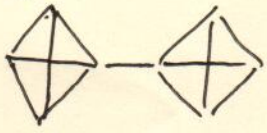
On a bipartite graph, a random walker simply jump alternatively from one set to another, therefore, it does not converge.

<u>Remark</u>. The values of λ_2, $\lambda_{|V|}$ are related to the convergence rate of a simple random walker to ~~the~~ its equilibrium state.

(II.2) <u>λ_2, Cheeger constant and connectedness</u>.

Recall G is connected $\Leftrightarrow \lambda_2 > 0$. Intutively, if G is connected but is very "close" to be disconnected, λ_2 should be close to 0. Can we find a quantitative description of this phenomena?

The first task is to quantify ~~the closeness~~ how much a graph is close to be disconnected.



G_1

G_2.

Intuitively, G_2 is "more" connected than G_1.

For any $\Omega \subset V$, we define $\mathrm{vol}(\Omega) := \sum_{x \in \Omega} d_x$.

We define the edge boundary of Ω to be

$$\partial\Omega = E(\Omega, \Omega^c) = \{ \{x,y\} \in E : x \in \Omega, y \in \Omega^c = V \setminus \Omega \}.$$

We denote $|\partial\Omega| = |E(\Omega, \Omega^c)|$ to be the cardinality of the boundary.

<u>Definition</u>: (Cheeger Constant): Given a finite simple graph $G = (V, E)$, its Cheeger constant is defined by

$$h = \inf_{\substack{\Omega \subset V \\ \mathrm{vol}(\Omega) \leq \frac{1}{2}\mathrm{vol}(G)}} \frac{|\partial\Omega|}{\mathrm{vol}(\Omega)}. \qquad \square$$

Remark (1). h is the largest constant s.t. the following inequality holds true:

$$|\partial\Omega| \geq h\, \mathrm{vol}(\Omega), \text{ for any } \Omega \subset V \text{ with } \mathrm{vol}(\Omega) \leq \tfrac{1}{2}\mathrm{vol}(G).$$

(2). An equivalent formulation of h is

$$h = \min_{\substack{(\Omega_1, \Omega_2) \\ \Omega_1 \sqcup \Omega_2 = V \\ \Omega_1, \Omega_2 \neq \phi}} \max_{i=1,2} \frac{|\partial\Omega_i|}{\mathrm{vol}(\Omega_i)}$$

For convenience, we denote by $\phi(\Omega) := \frac{|\partial\Omega|}{\mathrm{vol}(\Omega)}$.

<u>Theorem 2</u> [Alon-Milman '85, Dodziuk '84]. We have

$$\frac{h^2}{2} \leq \lambda_2 \leq 2h.$$

<u>Remark</u>: Recall $\lambda_2 = \min_{\substack{f \neq 0 \\ (f,1)=0}} R(f)$. In general, upper bound

estimate of λ_2 is easier since it usually reduce to a clever choice of function f s.t. $(f,1)=0$. In contrast, ~~the~~ lower bound estimates of λ_2 is harder.

<u>Proof of $\lambda_2 \leq 2h$</u>:

Let Ω be a subset of V s.t. $|\partial\Omega| = h\,\mathrm{vol}(\Omega)$.
$\mathrm{vol}(\Omega) \leq \frac{1}{2}\mathrm{vol}(G)$.

Consider
$$f(x) = \begin{cases} 1, & x \in \Omega \\ -a, & x \in \Omega^c \end{cases}$$

s.t. $(f,1)=0$. That is $\mathrm{vol}(\Omega) - a\,\mathrm{vol}(\Omega^c) = 0$, i.e.,
$$a = \frac{\mathrm{vol}(\Omega)}{\mathrm{vol}(\Omega^c)} \leq 1 \text{ by definition.}$$

Since $\lambda_2 \leq R(f)$, it remains to show $R(f) \leq 2h$.

We calculate $(f,f) = \mathrm{vol}(\Omega) + a^2\,\mathrm{vol}(\Omega^c) = (1+a)\,\mathrm{vol}(\Omega)$

and $(df,df) = \sum_{\{u,v\}\in E}(f(u)-f(v))^2 = \sum_{u\in\Omega}\sum_{\substack{v\in\Omega^c \\ v\sim u}}(f(u)-f(v))^2$

$$= (1+a)^2\,|\partial\Omega|.$$

Therefore, $R(f) = \dfrac{(1+a)^2|\partial\Omega|}{(1+a)\,\mathrm{vol}(\Omega)} = (1+a)\dfrac{|\partial\Omega|}{\mathrm{vol}(\Omega)} \leq 2\phi(\Omega) = 2h$. $\square$

<u>Proof of $\lambda_2 \geq \frac{h^2}{2}$</u>:

We divide our proof into two Lemmas. The first one reveals a deep relation between the Rayleigh Quotient of a function to ϕ.

<u>Lemma 1</u>. For any $g: V \to \mathbb{R}$, $\exists$ a subset $\Omega \subseteq \mathrm{supp}(g)$. with
$$\phi(\Omega) \leq \sqrt{2R(g)}.$$

<u>Lemma 2</u>: Let $\Delta f + \lambda_2 f = 0$. Then the function

$$g = f_+ := \begin{cases} f, & f \geq 0 \\ 0, & f < 0 \end{cases}$$

satisfies $\lambda_2 \geq R(g)$.

Proof of Lemma 1: We further restrict ourselves to the following family of subsets

$$\Omega_t := \{ x \in V : g(x)^2 > t \}, \quad t \in [0, \infty).$$

Our aim is to show

$$\frac{\int_0^\infty |\partial \Omega_t| \, dt}{\int_0^\infty \mathrm{vol}(\Omega_t) \, dt} \leq \sqrt{2R(g)}. \qquad (*)$$

$(*)$ implies there exists $t \in [0, \infty)$ for which $\phi(\Omega_t) \leq \frac{\int_0^\infty |\partial \Omega_t| \, dt}{\int_0^\infty \mathrm{vol}(\Omega_t) \, dt}$.

We calculate

$$\int_0^\infty \mathrm{vol}(\Omega_t) \, dt = \int_0^\infty \sum_{\substack{x \in V \\ g(x)^2 > t}} dx \, dt = \sum_{x \in V} \int_0^{g(x)^2} dt \, dx$$

$$= \sum_{x \in V} g(x)^2 \, dx = (g, g)$$

whereas

$$\int_0^\infty |\partial \Omega_t| \, dt = \int_0^\infty \sum_{\substack{\{u,v\} \in E \\ g(u)^2 > t \geq g(v)^2 \\ \text{or } g(u)^2 \leq t < g(v)^2}} 1 \, dt = \sum_{\{u,v\} \in E} \left| \int_{g(v)^2}^{g(u)^2} dt \right|$$

$$= \sum_{\{u,v\} \in E} | g(u)^2 - g(v)^2 |$$

$$= \sum_{\{u,v\} \in E} \left| (g(u) - g(v)) (g(u) + g(v)) \right|$$

$$\leq \sqrt{\sum_{\{u,v\} \in E} (g(u) - g(v))^2} \cdot \sqrt{\sum_{\{u,v\} \in E} (g(u) + g(v))^2}$$

$$\leq \sqrt{(dg,dg)} \cdot \sqrt{2\sum_{u\in V} g(u)^2 d_u} = \sqrt{(dg,dg)}\sqrt{2(g,g)}.$$

Therefore, we have

$$\frac{\int_0^\infty |\partial\Omega_t|\,dt}{\int_0^\infty \mathrm{vol}(\Omega_t)\,dt} \leq \frac{\sqrt{(dg,dg)}\sqrt{2(g,g)}}{(g,g)} = \sqrt{2R(g)}. \qquad \square.$$

<u>Proof of Lemma 2</u> : We observe that

$\lambda_2(f,g) = (-\Delta f, g) = (df, dg)$,

where $(f,g) = (g,g)$, (we use $a\cdot a_+ = a_+^2$ here)

and $$(df, dg) = \sum_{\{u,v\}\in E} (f(u)-f(v))(g(u)-g(v))$$

$$\geq \sum_{\{u,v\}\in E} (g(u)-g(v))^2 = (dg,dg)$$

(we use $|a_+ - b_+| \leq |a-b|$ and hence $|a_+-b_+|\,|a-b| \geq |a_+-b_+|^2$)

Therefore, we have $\lambda_2 = \dfrac{(df,dg)}{(f,g)} \geq \dfrac{(dg,dg)}{(g,g)} = R(g)$. $\square$.

<u>Proof of $\lambda_2 \geq \frac{h^2}{2}$</u> :

Let f be the eigenfct s.t. $\Delta f + \lambda_2 f = 0$.

Consider $\Omega_+ = \{x\in V : f(x) \geq 0\}$ and $\Omega_- = \{x\in V : f(x) < 0\}$.

W.l.o.g., we can assume $\mathrm{vol}(\Omega_+) \leq \frac{1}{2}\mathrm{vol}(V)$. (otherwise, use $-f$)

Let $g := f_+$. Then Lemma 1 & 2 together imply

$$\lambda_2 \geq R(g) \geq \frac{1}{2}\phi(\Omega_t)^2 \quad \text{for some } t\in[0,\infty)$$

and $\Omega_t := \{x\in V,\ g^2(x) > t\}$

since $\mathrm{vol}(\Omega_t) \leq \mathrm{vol}(\Omega_+) \leq \frac{1}{2}\mathrm{vol}(V)$

we arrive at $\lambda_2 \geq \frac{1}{2}\phi(\Omega_t)^2 \geq \frac{1}{2}h^2$. $\square$