图谱论组会讲稿 II

We shall discuss some subtle connections of spectral graph theory and classical analysis, including

- the Laplacian operator of a (simple) graph
- eigenvalue of weighted graphs
- application in theories of random walks

The Laplacian

> On the threshold of spectral graph analysis.

Laplatian operator of a graph

To begin with that, we shall review the definition of *adjacency matrix* $A(G)$ and *degree matrix* $D(G)$ for a simple graph G. The **Laplacian matrix**

$$L := D - A = \begin{cases} \deg v & u = v, \\ -1 & u \sim v, \\ 0 & \text{else.} \end{cases}$$

A brandnew concept named **Laplacian operator** (*Laplacian* for short) is defined as

$$\mathcal{L} := \begin{cases} 1 & u = v, \\ -\sqrt{\deg v \cdot \deg u}^{-1} & u \sim v, \\ 0 & \text{else.} \end{cases}$$

Here $\mathcal{L} = D^{-1/2} L D^{-1/2}$, where D^α is defined as

$$(\lambda_1^\alpha, \lambda_2^\alpha, \ldots, \lambda_k^\alpha, 0, \ldots, 0).$$

Consider the function $f : V(G) \to \mathbb{R}$ (or $\mathbb{C}$). Here we shall define the *inner product* ($\leftrightarrow$ what we done in *discrete Fourier analysis*).

$$\langle f, g \rangle := \sum_{v \in V} f(v) \overline{g(v)}$$

> For simplicity, we only discuss the real functions below.

Laplacian of a function can be also defined via the theorem of *unit decomposition*. Let δ_v be *characteristic function* w.r.t. v, then

$$\begin{aligned} \mathcal{L} f &= \sum_{v \in V} \langle \mathcal{L} f, \delta_v \rangle \cdot \delta_v \\ &= \sum_{v \in V} \sum_{u \in V} \left(f(u) - \sum_{u' \sim u} \frac{f(u')}{\sqrt{\deg u \cdot \deg u'}} \right) \delta_v(u) \cdot \delta_v \\ &= \sum_{v \in V} \frac{1}{\sqrt{\deg v}} \sum_{u \sim v} \left(\frac{f(v)}{\sqrt{\deg v}} - \frac{f(u)}{\sqrt{\deg u}} \right) \cdot \delta_v \end{aligned}$$

Hence $\forall v \in V$, we have

$$(\mathcal{L}f)(v) = \frac{1}{\sqrt{\deg v}} \sum_{u\sim v} \left(\frac{f(v)}{\sqrt{\deg v}} - \frac{f(u)}{\sqrt{\deg u}} \right).$$

Notice that $\mathcal{L} \sim \sum_i \partial_{x_i}(\partial x_i)$ in the continuous case in a *uniform-densitied* and *nongradient* medium.

Basic facts about eigenvalues

Suppose that λ is a eigenvalue of $\mathcal{L}$ w.r.t. some eigenfunction g, then

$$\frac{\langle g, \mathcal{L}g \rangle}{\langle g, g \rangle} = \lambda.$$

The L.H.S. outcomes

$$\frac{\langle g, \mathcal{L}g \rangle}{\langle g, g \rangle} = \frac{\sum_v \frac{g(v)}{\sqrt{\deg v}} \sum_{u\sim v} \left(\frac{g(v)}{\sqrt{\deg v}} - \frac{g(u)}{\sqrt{\deg u}} \right)}{\sum_v g(v)^2} =?$$

Whoops, how so? The dawn of victory might occur whence you think back

$$\langle f, Lf \rangle = \sum_{u\sim v} (f(v) - f(u))^2.$$

It suggests that once we substitude g with $T^{1/2}f$, we have

$$\frac{\langle g, \mathcal{L}g \rangle}{\langle g, g \rangle} = \frac{\sum_{u\sim v} (f(u) - f(v))^2}{\sum_v f(v)^2 \deg v}.$$

Furthermore, the laplacian is semi-positive since 0 is the smallest eigenvalue of L with corresponding eigenvector $\mathbf{1}_n$. Hence $T^{1/2}\mathbf{1}$ be an eigenfunction s.t.

$$\mathcal{L}(T^{1/2}\mathbf{1}) = T^{-1/2} L \mathbf{1}_n = 0.$$

> $\mathbf{1} : V \to \{1\}$ is constant function.

We call eigenvalue λ a main eigenvalue if and only if $\mathcal{E}_\lambda \not\subseteq \mathbf{1}^\perp$. The **spectra** of $\mathcal{L}$ are $0 \le \lambda_0 \le \lambda_1 \le \cdots \le \lambda_{n-1}$. We notice that the multiplicity of main eigenvalue 0 equals the number of *components* in G (trivial, but why?).

Hence λ_1 is defined as (notice that $\left\langle T^{1/2}f, T^{1/2}\mathbf{1} \right\rangle = 0$ while T is *self-adjoint*.)

$$\lambda_1 = \inf_{f \perp T\mathbf{1}} \frac{\sum_{u\sim v} (f(u) - f(v))^2}{\sum_v f(v)^2 \deg v}.$$

In continuous case... maybe we could steal a glance at the *Lichnerowicz–Obata theorem*. Let M denotes a compact Riemannian manifold without boundary. Consider the eigenfunction satisfying the equation $-\Delta u = \lambda u$, we obtain

$$\lambda \int_M u^2 = -\int_M (\Delta u) u = \int_M (\nabla u)^2.$$

Since the constant function is a trivial solution, the non-trivial solutions should be subject to $\int_M u = 0$. The function f s.t. $\left\langle T^{1/2}f, T^{1/2}\mathbf{1} \right\rangle = 0$ is also known as the **harmonic eigenfunction**.

Since $T^{1/2}f \perp T^{1/2}\mathbf{1}$, we can rewrite the expression of λ_1 into

$$\lambda_1 = \inf_f \sup_{t\in\mathbb{R}} \frac{\sum_{u\sim v}(f(u)-f(v))^2}{\sum_v (f(v)-t)^2 \deg v}.$$

whence the maximum holds, $2\sum_v (f(v)-t)\deg v = 0$. Let

$$\bar{f} := \frac{\sum_v f(v)\deg v}{\sum_v \deg v},$$

where $\sum_v \deg v = 2|E|$ is the **volume** of G. Notice that (why?)

$$\sum_v (f(v)-\bar{f})^2 \deg v = \sum_{u,v} (f(u)-f(v))^2 \deg u \deg v.$$

Hence

$$\lambda_1 = 2|E| \inf_f \frac{\sum_{u\sim v}(f(u)-f(v))^2}{\sum_{u\sim v}(f(u)-f(v))^2 \deg u \deg v}.$$

We can iterate the formula of *Rayleigh quotient* to get

$$\lambda_k = \inf_{f\perp T\cdot V_k} \frac{\sum_{u\sim v}(f(u)-f(v))^2}{\sum_v f(v)^2 \deg v}.$$

Here $V_k = \operatorname{span}\{\oplus_{i=0}^{k-1} x_k\}$, where x_k is the k-th eigenvector (notice that $\mathcal{L}$ is *diagonalisable*).

Spectrum of $\mathcal{L}$

For $K_{m,n}$, P_n, C_n, how to evaluate their eigenvalues and corresponding eigenvectors? Hint: using *Chebyshev polynomials* to evaluate the spectra of path and circles, deducing the corresponding eigenvectors by multiplying $(\alpha, \alpha^2, \ldots, \alpha^n)$.

As for graphs in general, some basic facts (bounds of eigenvalues) includes:

- $\sum_i \lambda_i \le n$, with equality holds $\Leftrightarrow$ G has no isolated points $\Leftrightarrow$ trace no less than n. Therefore, $\lambda_1 \le \dfrac{n}{n-1} \le \lambda_{n-1}$.
- $\lambda_1 \le 1$ when G is not complete (why?).
- $\lambda \le \sup_f \dfrac{\sum_{u\sim v}(f(u)-f(v))^2}{\sum_u f(u)^2 \deg u} \le \dfrac{2\sum_{u\sim v}(f(u)^2+f(v)^2)}{\sum_u f(u)^2 \deg u} \le 2.$

The equality in the last statement holds some non-trivial case. For instance, the following statements are equivalent (Hint: proof of connected case is sufficient enough; consider the eigen function $\mathbb{1}_A \cdot f(x) - \mathbb{1}_B \cdot f(x)$ for any bipartite with consisting part A and B):

1. G is bipartite.
2. $\lambda_{n-j} = 2$ if G has $i+1$ connected components.
3. For each λ_i, the value $2-\lambda_i$ is also an eigenvalue of G.

(Spectrum bounded by diameter and volume) Let D denotes the *diametre*. For $f \perp T\mathbf{1}$, let v_M be a vertex such that $|f(v_M)| = \max_v |f(v)|$. Since $\sum_v f(v)\deg v = 0$, there exists a u_0 such that $f(u_0)f(v_0) < 0$. Let P_{u_0,v_0} be the shortest *path* that connects u_0 and v_0, i.e.

$$v_0 - v_1 - \cdots - v_k = u_0.$$

Hence,

$$
\begin{aligned}
\lambda_1 &= \frac{\sum_{u\sim v}(f(u)-f(v))^2}{\sum_u f(u)^2 \deg u} \\
&\geq \frac{\sum_{i=1}^{k}(f(v_i)-f(v_{i-1}))^2}{f(v_0)^2\sum_u \deg u} \\
&\geq \frac{k\cdot\left(\dfrac{f(v_0)-f(v_k)}{k}\right)^2}{f(v_0)^2\sum_u \deg u} \\
&\geq \frac{1}{D\cdot\sum_u \deg u}
\end{aligned}
$$

A pure corollary deriving from $\mathcal{L}(\sqrt{T}f)=\lambda\sqrt{T}f$ is

$$
\lambda f(v)=\frac{1}{\deg v}\sum_{u\sim v}(f(u)-f(v))
$$

> Hint: Proof via $\mathcal{L}f=\lambda\sqrt{T}f$.

Spectrum of the weighted graphs

Denote w as a function defining *edge weights*, i.e.

$$
w: E\to\mathbb{R}, (u,v)\mapsto w(u,v).
$$

Here $w(u,v)=w(v,u)=w(e)$ is the weight of edge e between u and v.

Thence $\deg v=\sum_u w(u,v)$. In many cases of applications, the graph may equip with *self-loops* (any examples?). The Laplacian matrix is revised to be

$$
L:=D-A=\begin{cases}\deg v-w(v,v) & u=v,\\ -w(u,v) & u\sim v,\\ 0 & \text{else.}\end{cases}
$$

Hence

$$
\mathcal{L}:=\begin{cases}1-\dfrac{w(v,v)}{\deg v} & u=v,\\ -\dfrac{w(u,v)}{\sqrt{\deg v\cdot\deg u}} & u\sim v,\\ 0 & \text{else.}\end{cases}
$$

Similarly, some above-mentioned theorems are re-stated as:

- Here $\mathcal{L}=D^{-1/2}LD^{-1/2}$, where D^α is defined as

  $$
  (\lambda_1^\alpha,\lambda_2^\alpha,\ldots,\lambda_k^\alpha,0,\ldots,0).
  $$

- For $f:V\to\mathbb{R}$,

  $$
  Lf(v)=\sum_{u\sim v}(f(u)-f(v))w(u,v).
  $$

  Hence $\langle f,Lf\rangle=\sum_{u\sim v}(f(u)-f(v))^2w(u,v)$. λ_1
- Question: How to determine λ_k?