Introducing Spectral Graph Theory

We will be studying the spectra of *simple* graphs with no isolated points; that is, nondirected graphs without multiply-occurring edges or loops (i.e. edges with the same start and end vertex), and with at least one edge incident to each vertex.

The *combinatorial Laplacian* is given by

$$L(u,v) = \begin{cases} d_u \text{ if } u = v \\ -1 \text{ if } u \sim v \\ 0 \text{ if } u \not\sim v, u \neq v \end{cases}$$

while the *normalized Laplacian* is

$$\mathcal{L}(u,v) = \begin{cases} 1 \text{ if } u = v \\ \dfrac{-1}{\sqrt{d_u d_v}} \text{ if } u \sim v \\ 0 \text{ if } u \not\sim v, u \neq v \end{cases}$$

Note that $\mathcal{L} = D^{-\frac{1}{2}} L D^{-\frac{1}{2}}$.

Another relevant sort of matrix to graph properties is the probability matrix for a random walk, which is essentially a normalized form of the adjacency matrix:

$$P(u,v) = \begin{cases} \dfrac{1}{d_u} \text{ if } u \sim v \\ 0 \text{ if } u \not\sim v \end{cases}$$

Note that $P = D^{-1}A$, and, unlike A, is nonsymmetric.

The utility of P can be easily seen by considering the probabilities involved in a random walk: if we start, for instance, on the jth vertex, then after n steps our location probabilities are given by the vector $\begin{pmatrix} 0 & 0 & \cdots & 0 & 1 & 0 & \cdots & 0 & 0 \end{pmatrix} P^n$, with the one in the jth position of the first vector; in general, for an initial configuration f^* of points, we're interested in f^*P, f^*PP, f^*P^3, and so forth.

Clearly a relevant problem to this is how to calculate P^k efficiently; since P isn't even symmetric, diagonalization will be tricky. Our first simplification will be as such:

$$P^k = (D^{-1}A)^k = D^{-\frac{1}{2}}(D^{-\frac{1}{2}} A D^{-\frac{1}{2}})^k D^{\frac{1}{2}}$$

And we observe that the term $D^{-\frac{1}{2}} A D^{-\frac{1}{2}}$ (which we shall call $\mathcal{A}$) is symmetric, and is in fact simply $I - \mathcal{L}$, suggesting that the spectra of $\mathcal{A}$ and $\mathcal{L}$ are linked.

Furthermore, since $\mathcal{A}$ is symmetric, there is a unitary matrix U such that

$$\mathcal{A} = U \begin{pmatrix} \lambda_1 & & \\ & \ddots & \\ & & \lambda_n \end{pmatrix} U^{-1},$$

which is easy to raise to any power. The diagonal matrix herein consists of eigenvalues, so if we use eigenvectors as our basis for initial configurations, the eigenvalues of $\mathcal{A}$ (and the related vectors for $\mathcal{L}$) are clearly important.

Eigenvalues of $\mathcal{L}$

Since $\mathcal{L}$ is symmetric, its eigenvalues are real and non-negative. One eigenvalue is trivial: $\mathcal{L}$ has eigenvalue 0 associated with the vector $\varphi_0 = D^{\frac{1}{2}}\mathbf{1}$.

Finding the next-smallest eigenvalue is a matter of finding the smallest value of $\frac{\langle f,\mathcal{L}f\rangle}{\langle f,f\rangle}$ for f orthogonal to φ_0. Note that using the substitution $g = T^{-\frac{1}{2}}f$, we may rewrite the above as $\frac{\langle f,D^{-\frac{1}{2}}LD^{-\frac{1}{2}}f\rangle}{\langle f,f\rangle} = \frac{\langle g,Lg\rangle}{\langle T^{\frac{1}{2}}f,T^{\frac{1}{2}}f\rangle} = \frac{\sum_{u\sim v}(f(u)-f(v))^2}{\sum_v f(v)^2 d_v}$, so the first eigenvalue is given by

$$\lambda_1 = \inf_{f\perp\varphi_0} \frac{\langle f,\mathcal{L}f\rangle}{\langle f,f\rangle} = \inf_{f\perp\mathbf{1}} \frac{\sum_{u\sim v}(f(u)-f(v))^2}{\sum_v f(v)^2 d_v} = \inf_f \sup_C \frac{\sum_{u\sim v}(f(u)-f(v))^2}{\sum_v (f(v)-C)^2}$$

The penultimate formulation in tha above quotient is called the *Dirichlet sum*, and the last formulation is the *Raleigh quotient*.

Other eigenvalues can be obtained in a similar manner, but it is valuable, at this point, to ask what particular values of the eigenvalues signify. There are three straightforward results to be demonstrated:

Lemma 1. *If $\mathcal{L}$ has eigenvalues $0 = \lambda_0 \le \lambda_1 \le \cdots \le \lambda_{n-1}$, then it follows that*

1. *The number of zero eigenvalues is the number of components.*
2. $\lambda_{n-1} \le 2$.
3. $\lambda_{n-1} = 2$ *iff G is bipartite.*

Digression: Cutwidths and Bandwidths of $P\Box P$

We briefly study the question of finding $b(P\Box P)$ and $c(P\Box P)$ on the exam. The concepts of vertex boundary and edge boundary give us very good lower bounds on b and c:

Definition 1. The *vertex boundary* $\delta(S)$ of a subset S of the vertex set of a graph is $|\{v \in S : \exists u \in V(G) - S, v \sim u\}|$; that is, the vertex boundary is the number of points of S adjacent to points not in S.

Similarly, the *edge boundary* $\partial(S)$ of a subset S of the vertex set of a graph is $|\{(u,v) \in E(G) : u \in S, v \notin S\}|$; that is, the number of edges from points of S to points outside S.

The lower bounds follow straightforwardly that

$$b(G) \ge \max_k \min_{S\subseteq V(G),|S|=k} \delta(S)$$

$$c(G) \ge \max_k \min_{S\subseteq V(G),|S|=k} \partial(S)$$

since we can show that, if an embedding f assigns $\{1,\ldots,k\}$ to S, then $b(S) \ge \delta(S)$ and $c(S) \ge \partial(S)$.

Using this bound, it is easy to show that $b(P\Box P)$ and $c(P\Box P)$ are at least n, and embeddings which have bandwidths and cutwidths of n are attainable, so $b(P\Box P) = c(P\Box P) = n$.

Back to Eigenvalues

We still need to determine precisely what eigenvalues mean, however. If $\lambda_1 = 0$, we know G is not connected, but do particular nonzero λ_1 indicate anything? Basically, it indicates how bottlenecked the graph is: "wide" graphs tend to have higher λ_1 than "narrow ones". For instance, K_n, which is the widest graph possible, has all the nonzero eigenvalues clustered considerably higher. Similarly, the complete bipartite graph $K_{m,n}$ has all of its eigenvectors but the lowest and highest equal to 1. The cycle, which is a comparatively narrow graph, has eigenvalues $1 - \cos \frac{2\pi k}{n}$, which for large n has a very low λ_1. This seems to indicate an empirical meaning for λ_1, which we can explicitly describe.

Lemma 2. *If G is connected, then $\lambda_1 \geq \frac{1}{D(G)\,\mathrm{vol}(G)}$.*

Proof. By the Dirichlet sum,

$$\lambda_1 = \inf_{\sum_x f(x)d_x = 0} \frac{\sum_{x\sim y}(f(x) - f(y))^2}{\sum_x f^2(x)d_x}$$

Let ϕ be the function which yields the infimum above. Let us choose v to maximize $M = |\phi(v)|$, and let v' be a point such that $\phi(v)$ and $\phi(v')$ are of opposite signs. By connectedness, there is a path P from v to v' of length no greater than $D(G)$. Then

$$\begin{aligned} \lambda_1 &= \frac{\sum_{x\sim y}(\phi(x) - phi(y))^2}{\sum_x \phi^2(x)d_x} \\ &\geq \frac{\sum_{(x,y)\in P}(\phi(x) - phi(y))^2}{M^2 \sum_x d_x} \end{aligned}$$

Noting that $\sum_{i=1}^n a_i^2 \geq \frac{1}{n}\left(\sum_{i=1}^n a_i\right)^2$, it is the case that

$$\begin{aligned} \lambda_1 &\geq \frac{\frac{1}{D(G)}\left(\sum_{(x,y)\in P} \phi(x) - phi(y)\right)^2}{M^2\,\mathrm{vol}(G)} \\ &\geq \frac{(\phi(v) - phi(v'))^2}{D(G)M^2\,\mathrm{vol}(G)} \\ &\geq \frac{M^2}{D(G)M^2\,\mathrm{vol}(G)} \geq \frac{1}{D(G)\,\mathrm{vol}(G)} \end{aligned}$$

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