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Spectral Graph Theory

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Abstract

Spectral graph theory deals with the eigenvalues of a graph. The set of eigenvalues of a graph, is referred to, as the spectrum of the associated graph. The spectrum has indeed many important applications in graph theory. I will address some of these applications, but there are many more.

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Chapter 1

Eigenvalues and the Laplacian of a graph

1.1 The Laplacian and eigenvalues

We begin with a graph G . Let d_v denote the degree of the vertex v . The first step is to define the Laplacian for graphs without loops and multiple edges. Consider the matrix L , defined as:

$$L(u, v) = \begin{cases} d_v & \text{if } u = v \\ -1 & \text{if } u \text{ and } v \text{ are adjacent} \\ 0 & \text{otherwise} \end{cases}$$

Then we define the *Laplacian* of G as the matrix:

$$\mathcal{L}(u, v) = \begin{cases} 1 & \text{if } u = v \text{ and } d_v \neq 0 \\ -\frac{1}{\sqrt{d_u d_v}} & \text{if } u \text{ and } v \text{ are adjacent} \\ 0 & \text{otherwise} \end{cases}$$

T denotes the diagonal matrix with the (v, v) -th entry having value d_v . We can write

$$\mathcal{L} = T^{-1/2} L T^{-1/2}$$

where $T^{-1}(v, v) = 0$ for $d_v = 0$. (Notice that if $d_v = 0$, the vertex v is isolated.) A graph is called nontrivial if it contains at least one edge.

The matrix \mathcal{L} can be viewed as an operator on the space of functions $g : V(G) \rightarrow \mathbb{R}$ which satisfies

$$\mathcal{L}(g(u)) = \frac{1}{\sqrt{d_u}} \sum_{v \sim u} \left(\frac{g(u)}{\sqrt{d_u}} - \frac{g(v)}{\sqrt{d_v}} \right)$$

Where $\sum_{u \sim v}$ denotes the sum over all unordered pairs $\{u, v\}$ for which u and v are adjacent. When G is k -regular, i.e. every vertex has degree k , we have

$$\mathcal{L} = I - \frac{1}{k} A,$$

where A is the usual adjacency matrix of G and I is the identity matrix. The matrices here are $n \times n$ where n is the number of vertices in G . For a general graph, we have

$$\mathcal{L} = T^{-1/2}LT^{-1/2} = I - T^{-1/2}AT^{-1/2}.$$

Moreover, \mathcal{L} can be written as

$$\mathcal{L} = SS^t,$$

where in the matrix S the rows are indexed by the vertices and the columns are indexed by the edges of G . Each column that corresponds to an edge $e = \{u, v\}$ has an entry $\frac{1}{\sqrt{d_u}}$ in the row corresponding to u , an entry $\frac{1}{\sqrt{d_v}}$ in the row corresponding to v , and has zero entries elsewhere.

The eigenvalues of \mathcal{L} are all real and non-negative, since \mathcal{L} is symmetric. When we have these characterizations of the eigenvalues, we can use the Rayleigh quotient of \mathcal{L} . The Rayleigh quotient is used in eigenvalue algorithms to obtain an eigenvalue from an eigenvector. Let g be an arbitrary function which assigns a real number $g(v)$ to each vertex v of G and g can be viewed as a column vector. Then, one has

$$\begin{aligned} \frac{\langle g, \mathcal{L}g \rangle}{\langle g, g \rangle} &= \frac{\langle g, T^{-1/2}LT^{-1/2}g \rangle}{\langle g, g \rangle} = \\ &= \frac{\langle f, Lf \rangle}{\langle T^{1/2}f, T^{1/2}f \rangle} = \\ &= \frac{\sum_{u \sim v} (f(u) - f(v))^2}{\sum_v f(v)^2 d_v} \end{aligned} \tag{1.1}$$

where $g = T^{1/2}f$ and $\sum_{u \sim v}$ denotes the sum over all unordered pairs $\{u, v\}$ for which u and v are adjacent. $\sum_{u \sim v} (f(u) - f(v))^2$ is called the *Dirichlet sum* of G and the ratio in the left hand side of (1.1) is called the *Rayleigh quotient*.

According to equation (1.1) all eigenvalues are non-negative and we deduce that 0 is an eigenvalue of \mathcal{L} , as our next example will demonstrate. We denote the eigenvalues of \mathcal{L} by $0 = \lambda_0 \leq \lambda_1 \leq \dots \leq \lambda_{n-1}$. Since \mathcal{L} is symmetric, \mathcal{L} has an orthogonal basis of eigenvectors. The *spectrum* of \mathcal{L} is the set of the λ_i 's. Let $\mathbf{1}$ denote the constant function which assumes the value 1 on each vertex. Then $T^{1/2}\mathbf{1}$ is an eigenfunction of \mathcal{L} with eigenvalue 0. We also have

$$\lambda_G = \lambda_1 = \inf_{f \perp T\mathbf{1}} \frac{\sum_{u \sim v} (f(u) - f(v))^2}{\sum_v f(v)^2 d_v}. \tag{1.2}$$

The corresponding eigenfunction is $g = T^{1/2}f$ as in (1.1). The function f in (1.2) is a function called a *harmonic eigenfunction* of \mathcal{L} .

The above definition for λ_G corresponds to the eigenvalues of the Laplace-Beltrami operator for Riemannian manifolds: $\lambda_M = \inf \frac{\int_M |\nabla f|^2}{\int_M |f|^2}$ where f ranges over functions satisfying $\int_M f = 0$

Example 1.1 The eigenvalues for a complete graph K_3 on 3 vertices, are determined in the following way:

We begin with $g = T^{1/2}\mathbf{1}$ and since $f = T^{-1/2}g$, we have $f = \mathbf{1} = (1, 1, 1)$. Then, one has

$$\begin{aligned} \lambda_0 &= \frac{\sum_{u \sim v} (f(u) - f(v))^2}{\sum_v f(v)^2 d_v} = \\ &= \frac{\left(\langle(1, 1, 1), (1, 0, 0)\rangle - \langle(1, 1, 1), (0, 1, 0)\rangle\right)^2 + \left(\langle(1, 1, 1), (0, 1, 0)\rangle - \langle(1, 1, 1), (0, 0, 1)\rangle\right)^2 + \\ &\quad \left(\langle(1, 1, 1), (0, 1, 0)\rangle\right)^2 \cdot 2 + \left(\langle(1, 1, 1), (0, 0, 1)\rangle\right)^2 \cdot 2 + \\ &\quad + \left(\langle(1, 1, 1), (0, 0, 1)\rangle - \langle(1, 1, 1), (1, 0, 0)\rangle\right)^2}{\left(\langle(1, 1, 1), (0, 1, 0)\rangle\right)^2 \cdot 2 + \left(\langle(1, 1, 1), (0, 0, 1)\rangle\right)^2 \cdot 2 + \\ &\quad + \left(\langle(1, 1, 1), (1, 0, 0)\rangle\right)^2 \cdot 2} = \frac{(1-1)^2 + (1-1)^2 + (1-1)^2}{1^2 \cdot 2 + 1^2 \cdot 2 + 1^2 \cdot 2} = 0 \end{aligned}$$

To get λ_1 we use equation (1.2), where f must be orthogonal to $T\mathbf{1}$. $T\mathbf{1} = (2, 2, 2)$. $(-2, 2, 0)$ is orthogonal to $(2, 2, 2)$. Then, one has

$$\begin{aligned} \lambda_1 &= \inf_{f \perp T\mathbf{1}} \frac{\sum_{u \sim v} (f(u) - f(v))^2}{\sum_v f(v)^2 d_v} = \\ &= \frac{\left(\langle(-2, 2, 0), (1, 0, 0)\rangle - \langle(-2, 2, 0), (0, 1, 0)\rangle\right)^2 + \left(\langle(-2, 2, 0), (0, 1, 0)\rangle - \langle(-2, 2, 0), (0, 0, 1)\rangle\right)^2 + \\ &\quad \left(\langle(-2, 2, 0), (0, 1, 0)\rangle\right)^2 \cdot 2 + \left(\langle(-2, 2, 0), (0, 0, 1)\rangle\right)^2 \cdot 2 + \\ &\quad + \left(\langle(-2, 2, 0), (0, 0, 1)\rangle - \langle(-2, 2, 0), (1, 0, 0)\rangle\right)^2}{\left(\langle(-2, 2, 0), (0, 1, 0)\rangle\right)^2 \cdot 2 + \left(\langle(-2, 2, 0), (0, 0, 1)\rangle\right)^2 \cdot 2 + \\ &\quad + \left(\langle(-2, 2, 0), (1, 0, 0)\rangle\right)^2 \cdot 2} = \frac{(-2-2)^2 + (2-0)^2 + (0-(-2))^2}{2^2 \cdot 2 + 0^2 \cdot 2 + (-2)^2 \cdot 2} = \\ &= \frac{16 + 4 + 4}{8 + 8} = \frac{24}{16} = \frac{3}{2} \end{aligned}$$

To get λ_2 , f must be orthogonal to both $(2, 2, 2)$ and $(-2, 2, 0)$. $(2, 2, -4)$ is such a

vector, which generates a basis of eigenvectors. Then, one has

$$\begin{aligned}
\lambda_2 &= \sup_f \frac{\sum_{u \sim v} (f(u) - f(v))^2}{\sum_v f(v)^2 d_v} = \\
&= \frac{\left(\langle (2, 2, -4), (1, 0, 0) \rangle - \langle (2, 2, -4), (0, 1, 0) \rangle \right)^2 + \left(\langle (2, 2, -4), (0, 1, 0) \rangle - \langle (2, 2, -4), (0, 0, 1) \rangle \right)^2 + \\
&\quad \left(\langle (2, 2, -4), (0, 1, 0) \rangle \right)^2 \cdot 2 + \left(\langle (2, 2, -4), (0, 0, 1) \rangle \right)^2 \cdot 2 + \\
&\quad + \left(\langle (2, 2, -4), (0, 0, 1) \rangle - \langle (2, 2, -4), (1, 0, 0) \rangle \right)^2}{\left(\langle (2, 2, -4), (1, 0, 0) \rangle \right)^2 \cdot 2 + \left(\langle (2, 2, -4), (0, 1, 0) \rangle \right)^2 \cdot 2 + \\
&\quad + \left(\langle (2, 2, -4), (0, 0, 1) \rangle - \langle (2, 2, -4), (1, 0, 0) \rangle \right)^2} = \frac{(2-2)^2 + (2-(-4))^2 + (-4-2)^2}{2^2 \cdot 2 + (-4)^2 \cdot 2 + 2^2 \cdot 2} = \\
&= \frac{0 + 36 + 36}{8 + 32 + 8} = \frac{72}{48} = \frac{3}{2}
\end{aligned}$$

So the eigenvalues are $\lambda_0 = 0$, $\lambda_1 = 3/2$ and $\lambda_2 = 3/2$. □

We can express (1.2) in several ways:

$$\lambda_1 = \inf_f \sup_t \frac{\sum_{u \sim v} (f(u) - f(v))^2}{\sum_v (f(v) - t)^2 d_v} = \tag{1.3}$$

$$= \inf_f \frac{\sum_{u \sim v} (f(u) - f(v))^2}{\sum_v (f(v) - \bar{f})^2 d_v} \tag{1.4}$$

where $\bar{f} = \frac{\sum_v f(v) d_v}{\text{vol } G}$ and $\text{vol } G$ denotes the volume of the graph G , given by

$$\text{vol } G = \sum_v d_v.$$

By substituting for \bar{f} and using $N \sum_{i=1}^N (a_i - a)^2 = \sum_{i < j} (a_i - a_j)^2$ for

$a = \sum_{i=1}^N a_i / N$, we have the following expression:

$$\lambda_1 = \text{vol } G \inf_f \frac{\sum_{u \sim v} (f(u) - f(v))^2}{\sum_{u, v} (f(u) - f(v))^2 d_u d_v} \tag{1.5}$$

where $\sum_{u, v}$ denotes the sum over all unordered pairs of vertices u, v in G . The other eigenvalues of \mathcal{L} can be characterized in terms of the Rayleigh quotient.

The largest eigenvalue satisfies:

$$\lambda_{n-1} = \sup_f \frac{\sum_{u \sim v} (f(u) - f(v))^2}{\sum_v f^2(v) d_v} \quad (1.6)$$

For a general k , one has:

$$\lambda_k = \inf_f \sup_{g \in P_{k-1}} \frac{\sum_{u \sim v} (f(u) - f(v))^2}{\sum_v (f(v) - g(v))^2 d_v} = \quad (1.7)$$

$$= \inf_{f \perp TP_{k-1}} \frac{\sum_{u \sim v} (f(u) - f(v))^2}{\sum_v f^2(v) d_v} \quad (1.8)$$

where P_i is the subspace generated by the harmonic eigenfunctions corresponding to λ_i for $i \leq k - 1$.

Example 1.2 The eigenvalues for a complete graph K_n on n vertices, are 0 and $n/(n - 1)$ (with multiplicity $n - 1$).

Example 1.3 The eigenvalues for a complete bipartite graph $K_{m,n}$ on $m + n$ vertices, are 0,1 (with multiplicity $m + n - 2$), and 2.

Example 1.4 The eigenvalues for a star S_n on n vertices, are 0,1 (with multiplicity $n - 2$), and 2.

1.2 The spectrum of a graph

The main problems of spectral theory lie in deriving bounds on the distributions of eigenvalues and the impact and consequences of the eigenvalue bounds as well as their applications. In this section we state some simple lower and upper bounds of the eigenvalues. We will see that the eigenvalues of any graph lie between 0 and 2.

Lemma 1.1: *For a graph G on n vertices, we have*

(i)

$$\sum_i \lambda_i \leq n$$

with equality holding if and only if G has no isolated vertices.

(ii) For $n \geq 2$, one has

$$\lambda_1 \leq \frac{n}{n-1}$$

with equality holding if and only if G is the complete graph on vertices. Also, for a graph G without isolated vertices, we have

$$\lambda_{n-1} \geq \frac{n}{n-1}.$$

- (iii) For a graph different from a complete graph, we have $\lambda_1 \leq 1$.
- (iv) If G is connected, then $\lambda_1 > 0$. If $\lambda_i = 0$ and $\lambda_{i+1} \neq 0$, then G has exactly $i + 1$ connected components.
- (v) For all $i \leq n - 1$, we have $\lambda_i \leq 2$ with $\lambda_{n-1} = 2$ if and only if a connected component of G is bipartite and nontrivial.
- (vi) The spectrum of a graph is the union of the spectra of its connected components.

Proof: (i) follows from considering the trace of \mathcal{L} . (The trace of an n by n square matrix is defined to be the sum of the elements on the main diagonal.)

The inequalities in (ii) follow from (i) and $\lambda_0 = 0$.

Suppose G contains two nonadjacent vertices a and b , and consider

$$f_1(v) = \begin{cases} d_b & \text{if } v = a \\ -d_a & \text{if } v = b \\ 0 & \text{if } v \neq a, b. \end{cases}$$

(iii) then follows from (1.2).

If G is connected, the eigenvalue 0 has multiplicity 1 since any harmonic eigenfunction (1.2) with eigenvalue 0 assumes the same value at each vertex. Thus, (iv) follows from the fact that the union of two disjoint graphs has as its spectrum the union of the spectra of the original graphs.

(v) follows from equation (1.6) and the fact that

$$(f(x) - f(y))^2 \leq 2(f^2(x) + f^2(y)).$$

Therefore

$$\lambda_i \leq \sup_f \frac{\sum_{x \sim y} (f(x) - f(y))^2}{\sum_x f^2(x) d_x} \leq 2.$$

Equality holds for $i = n - 1$ when $f(x) = -f(y)$ for every edge $\{x, y\}$ in G . Therefore, since $f \neq 0$, G has a bipartite connected component. On the other hand, if G has a connected component which is bipartite, we can choose the function f so as to make $\lambda_{n-1} = 2$.

(vi) follows from the definition. □

For bipartite graphs, the following slightly stronger result holds:

Lemma 1.2: *The following statements are equivalent:*

(i): G is bipartite.

(ii): G has $i + 1$ connected components and $\lambda_{n-j} = 2$ for $1 \leq j \leq i$.

(iii): For each λ_i , the value $2 - \lambda_i$ is also an eigenvalue of G .

Proof: It suffices to consider a connected graph. Suppose G is a bipartite graph with vertex set consisting of two parts A and B . For any harmonic eigenfunction f with eigenvalue λ , we consider the function g

$$g(x) = \begin{cases} f(x) & \text{if } x \in A, \\ -f(x) & \text{if } x \in B. \end{cases}$$

It is easy to check that g is a harmonic eigenfunction with eigenvalue $2 - \lambda$. □

The *distance* between two vertices u and v is the number of edges in a shortest path joining u and v . The maximum distance between any two vertices of G is the *diameter* of a graph. Here we will give, for a connected graph, a simple eigenvalue lower bound in terms of the diameter of a graph.

Lemma 1.3: For a connected graph G with diameter D , we have

$$\lambda_1 \geq \frac{1}{D \operatorname{vol} G}.$$

Proof: Suppose f is a harmonic eigenfunction achieving λ_1 in (1.2). Let v_0 denote a vertex with $|f(v_0)| = \max_v |f(v)|$. Since $\sum_{u,v} f(v) = 0$, there exists a vertex u_0 satisfying $f(u_0)f(v_0) \leq 0$. Let P denote a shortest path in G joining u_0 and v_0 . Then by (1.2) we have

$$\begin{aligned} \lambda_1 &= \frac{\sum_{x \sim y} (f(x) - f(y))^2}{\sum_x f^2(x) d_x} \geq \\ &\geq \frac{\sum_{\{x,y\} \in P} (f(x) - f(y))^2}{\operatorname{vol} G f^2(v_0)} \geq \\ &\geq \frac{\frac{1}{D} (f(v_0) - f(u_0))^2}{\operatorname{vol} G f^2(v_0)} \geq \\ &\geq \frac{1}{D \operatorname{vol} G} \end{aligned}$$

by using the Cauchy-Schwarz inequality. □

Lemma 1.4: Let f denote a harmonic eigenfunction achieving λ_G in (1.2). Then, for any vertex $x \in V$, we have

$$\frac{1}{d_x} \sum_{\substack{y \\ y \sim x}} (f(x) - f(y)) = \lambda_G f(x).$$

Proof: We use a variational argument. For a fixed $x_0 \in V$, we consider f_ϵ such that

$$f_\epsilon(y) = \begin{cases} f(x_0) + \frac{\epsilon}{d_{x_0}} & \text{if } y = x_0 \\ f(y) - \frac{\epsilon}{\text{vol } G - d_{x_0}} & \text{otherwise.} \end{cases}$$

We have

$$\begin{aligned} & \frac{\sum_{\substack{x, y \in V \\ x \sim y}} (f_\epsilon(x) - f_\epsilon(y))^2}{\sum_{x \in V} f_\epsilon^2(x) d_x} = \\ &= \frac{\sum_{\substack{x, y \in V \\ x \sim y}} (f(x) - f(y))^2 + \sum_{\substack{y \\ y \sim x_0}} \frac{2\epsilon(f(x_0) - f(y))}{d_{x_0}} - \sum_{\substack{y \\ y \neq x_0}} \sum_{\substack{y' \\ y \sim y'}} \frac{2\epsilon(f(y) - f(y'))}{\text{vol } G - d_{x_0}}}{\sum_{x \in V} f^2(x) d_x + 2\epsilon f(x_0) - \frac{2\epsilon}{\text{vol } G - d_{x_0}} \sum_{y \neq x_0} f(y) d_y} + O(\epsilon^2) = \\ &= \frac{\sum_{\substack{x, y \in V \\ x \sim y}} (f(x) - f(y))^2 + \frac{2\epsilon \sum_{\substack{y \\ y \sim x_0}} (f(x_0) - f(y))}{d_{x_0}} + \frac{2\epsilon \sum_{\substack{y \\ y \sim x_0}} (f(x_0) - f(y))}{\text{vol } G - d_{x_0}}}{\sum_{x \in V} f^2(x) d_x + 2\epsilon f(x_0) + \frac{2\epsilon f(x_0) d_{x_0}}{\text{vol } G - d_{x_0}}} + O(\epsilon^2) \end{aligned}$$

since $\sum_{x \in V} f(x) d_x = 0$, and $\sum_y \sum_{y'} (f(y) - f(y')) = 0$. The definition in (1.2) implies that

$$\frac{\sum_{\substack{x, y \in V \\ x \sim y}} (f_\epsilon(x) - f_\epsilon(y))^2}{\sum_{x \in V} f_\epsilon^2(x) d_x} \geq \frac{\sum_{\substack{x, y \in V \\ x \sim y}} (f(x) - f(y))^2}{\sum_{x \in V} f^2(x) d_x}.$$

If we consider what happens to the Rayleigh quotient for f_ϵ as $\epsilon \rightarrow 0 \pm$ we can conclude that

$$\frac{1}{d_{x_0}} \sum_{\substack{y \\ y \sim x_0}} (f(x_0) - f(y)) = \lambda_G f(x_0)$$

and the Lemma is proved. \square

Lemma 1.4 can also be proved by using that $f = T^{-1/2}g$, where $\mathcal{L}g = \lambda_G g$. Then $T^{-1}Lf = T^{-1}(T^{1/2}\mathcal{L}T^{1/2})(T^{-1/2}g) = T^{-1/2}\lambda_G g = \lambda_G f$, and examining the entries gives the desired result.

Using linear algebra, the bounds on eigenvalues in terms of the degrees of the vertices can be improved. Consider the trace of $(I - \mathcal{L})^2$. We have

$$\begin{aligned} \text{Tr}(I - \mathcal{L})^2 &= \sum_i (1 - \lambda_i)^2 \leq \\ &\leq 1 + (n-1)\bar{\lambda}^2, \end{aligned} \quad (1.9)$$

where $\bar{\lambda} = \max_{i \neq 0} |1 - \lambda_i|$. On the other hand,

$$\begin{aligned} \text{Tr}(I - \mathcal{L})^2 &= \text{Tr}(T^{-1/2}AT^{-1}AT^{-1/2}) = \\ &= \sum_{x,y} \frac{1}{\sqrt{d_x}} A(x,y) \frac{1}{d_y} A(y,x) \frac{1}{\sqrt{d_x}} = \\ &= \sum_x \frac{1}{d_x} - \sum_{x \sim y} \left(\frac{1}{d_x} - \frac{1}{d_y} \right)^2, \end{aligned} \quad (1.10)$$

where A is the adjacency matrix. From this, we deduce

Lemma 1.5: *For a k -regular graph G on n vertices, we have*

$$\max_{i \neq 0} |1 - \lambda_i| \geq \sqrt{\frac{n-k}{(n-1)k}}. \quad (1.11)$$

This follows from the fact that $\max_{i \neq 0} |1 - \lambda_i|^2 \geq \frac{1}{n-1} (\text{Tr}(I - \mathcal{L})^2 - 1)$.

Let d_H denote the harmonic mean of the d_v 's, then $\frac{1}{d_H} = \frac{1}{n} \sum_v \frac{1}{d_v}$. For a general graph we can use the fact that

$$\frac{\sum_{x \sim y} \left(\frac{1}{d_x} - \frac{1}{d_y} \right)^2}{\sum_{x \in V} \left(\frac{1}{d_x} - \frac{1}{d_H} \right)^2 d_x} \leq \lambda_{n-1} \leq 1 + \bar{\lambda}. \quad (1.12)$$

Combining (1.9), (1.10) and (1.12), we obtain:

Lemma 1.6: *For a graph G on n vertices, $\bar{\lambda} = \max_{i \neq 0} |1 - \lambda_i|$ satisfies the inequality $1 + (n-1)\bar{\lambda}^2 \geq \frac{n}{d_H} (1 - (1 + \bar{\lambda}) \left(\frac{k}{d_H} - 1 \right))$, where k denotes the average degree of G .*

We can choose any function $f : V(G) \rightarrow \mathbb{R}$ from the characterization in the preceding section and its Rayleigh quotient will serve as an upper bound for λ_1 .

Here we describe an upper bound for λ_1 .

Lemma 1.7: *Let G be a graph with diameter $D \geq 4$, and let k denote the maximum degree of G . Then $\lambda_1 \leq 1 - 2\frac{\sqrt{k-1}}{k}\left(1 - \frac{2}{D}\right) + \frac{2}{D}$.*

Lemma 1.7 will be proved in the next section. One way to bound eigenvalues from above is to consider "contraction" of the graph G into a weighted graph H (which will be defined in the next section). Then the eigenvalues of G can be upper-bounded by the eigenvalues of H or by various upper bounds on them, which might be easier to obtain. The proof of Lemma 1.7 proceeds by contracting the graph into a weighted path. Lemma 1.7 gives a proof that for any fixed k and for any infinite family of regular graphs with degree k , one has $\limsup \lambda_1 \leq 1 - 2\frac{\sqrt{k-1}}{k}$.

1.3 Eigenvalues of weighted graphs

All definitions and subsequent theorems for simple graphs can usually be easily carried out for weighted graphs. A weighted undirected graph G has associated with it a weight function $w : V \times V \rightarrow \mathbb{R}$ satisfying $w(u, v) = w(v, u)$ and $w(u, v) \geq 0$. If $\{u, v\} \notin E(G)$. Then $w(u, v) = 0$. Unweighted graphs are the special case where all the weights are 0 or 1. Here we define the degree d_v of a vertex v as $d_v = \sum_u w(u, v)$ and $\text{vol } G = \sum_v d_v$. The definitions of previous sections can be generalized as $L(u, v) = \begin{cases} d_v - w(v, v) & \text{if } u = v \\ -w(u, v) & \text{if } u \text{ and } v \text{ are adjacent} \\ 0 & \text{otherwise.} \end{cases}$

For a function $f : V \rightarrow \mathbb{R}$ we have $L(f(x)) = \sum_{x \sim y} (f(x) - f(y))w(x, y)$.

Let T denote the diagonal matrix with the (v, v) -th entry having value d_v . The Laplacian of G is defined to be $\mathcal{L} = T^{-1/2}LT^{-1/2}$. We have

$$\mathcal{L}(u, v) = \begin{cases} 1 - \frac{w(v, v)}{d_v} & \text{if } u = v \text{ and } d_v \neq 0 \\ -\frac{w(u, v)}{\sqrt{d_u d_v}} & \text{if } u \text{ and } v \text{ are adjacent} \\ 0 & \text{otherwise.} \end{cases}$$

The same characterizations for the eigenvalues of the generalized versions of

\mathcal{L} can still be used. For example:

$$\begin{aligned}
\lambda_G := \lambda_1 &= \inf_{g \perp T^{1/2} \mathbf{1}} \frac{\langle g, \mathcal{L}g \rangle}{\langle g, g \rangle} = & (1.13) \\
&= \inf_{\sum f(x)d_x=0} \frac{\sum_{x \in V} f(x)Lf(x)}{\sum_{x \in V} f^2(x)d_x} = \\
&= \inf_{\sum f(x)d_x=0} \frac{\sum_{x \sim y} (f(x) - f(y))^2 w(x, y)}{\sum_{x \in V} f^2(x)d_x}.
\end{aligned}$$

If we identify two distinct vertices, say u and v , into a single vertex v^* we form a contraction of a graph G . The weights of edges incident to v^* are defined as follows:

$$\begin{aligned}
w(x, v^*) &= w(x, u) + w(x, v) \\
w(v^*, v^*) &= w(u, u) + w(v, v) + 2w(u, v).
\end{aligned}$$

Lemma 1.8: *If H is formed by contractions from a graph G , then $\lambda_G \leq \lambda_H$.*

The proof follows from the fact that an eigenfunction which achieves λ_H for H can be lifted to a function defined on $V(G)$ such that all vertices in G that contract to the same vertex in H share the same value.

We return to Lemma 1.7.

Proof of lemma 1.7: Let u, v denote two vertices that are at distance $D \geq 2t + 2$ in G . We contract G into a path H with $2t + 2$ edges, with vertices $x_0, x_1, \dots, x_t, z, y_t, \dots, y_2, y_1, y_0$ such that vertices at distance i from u , $0 \leq i \leq t$, are contracted to x_i , and vertices at distance j from v , $0 \leq j \leq t$, are contracted to y_j . The remaining vertices are contracted to z . To establish an upper bound for λ_1 , it is enough to choose a suitable function f , defined as follows:

$$\begin{aligned}
f(x_i) &= a(k-1)^{-i/2} \\
f(y_j) &= b(k-1)^{-j/2} \\
f(z) &= 0,
\end{aligned}$$

where the constants a and b are chosen to achieve $\sum_x f(x)d_x = 0$. It can be checked that the Rayleigh quotient satisfies

$$\frac{\sum_{u \sim v} (f(u) - f(v))^2 w(u, v)}{\sum_v f(v)^2 d_v} \leq 1 - \frac{2\sqrt{k-1}}{k} \left(1 - \frac{1}{t+1}\right) + \frac{1}{t+1},$$

since the ratio is maximized when $w(x_i, x_{i+1}) = k(k-1)^{i-1} = w(y_i, y_{i+1})$. This completes the proof of the lemma. □

Chapter 2

The Cheeger constant and the edge expansion of a graph

2.1 The Cheeger constant of a graph

Let us define measure on subsets of vertices by taking the degree of a vertex into consideration. For a subset S of the vertices of G , we define $\text{vol } S$, the *volume* of S , to be the degrees of the vertices in S : $\text{vol } S = \sum_{x \in S} d_x$, for $S \subseteq V(G)$.

We define the *edge boundary* ∂S of S to consist of all edges with exactly one endpoint in S :

$$\partial S = \{\{u, v\} \in E(G) : u \in S \text{ and } v \notin S\}.$$

\bar{S} denotes the complement of S . So $\bar{S} = V - S$ and $\partial S = \partial \bar{S} = E(S, \bar{S})$ where $E(A, B)$ denotes the set of edges with one endpoint in A and one endpoint in B . The *vertex boundary* δS of S is defined to be the set of all vertices v not in S but adjacent to some vertex in S :

$$\delta S = \{v \notin S : \{u, v\} \in E(G), u \in S\}.$$

Some questions:

Problem 1: For a fixed number m , find a subset S with $m \leq \text{vol } S \leq \text{vol } \bar{S}$ such that the edge boundary ∂S contains as few edges as possible.

Problem 2: For a fixed number m , find a subset S with $m \leq \text{vol } S \leq \text{vol } \bar{S}$ such that the vertex boundary δS contains as few vertices as possible.

Cheeger constants are meant to answer exactly the questions above. For a subset $S \subset V$ we define

$$h_G(S) = \frac{|E(S, \bar{S})|}{\min(\text{vol } S, \text{vol } \bar{S})}. \quad (2.1)$$

The Cheeger constant h_G of a graph G is defined to be

$$h_G = \min_S h_G(S). \quad (2.2)$$

The problem of determining the Cheeger constant is in some sense equivalent to solving Problem 1, since $|\partial S| \geq h_G \text{vol } S$.

G is connected if and only if $h_G > 0$. We will only consider connected graphs. We define the analogue of (2.1) for vertex expansion. For a subset $S \subseteq V$, we define

$$g_G(S) = \frac{\text{vol } \delta(S)}{\min(\text{vol } S, \text{vol } \bar{S})} \quad (2.3)$$

and

$$g_G = \min_S g_G(S). \quad (2.4)$$

For regular graphs, we have $g_G(S) = \frac{|\delta(S)|}{\min(|S|, |\bar{S}|)}$.

We can define a modified Cheeger constant if we decide to have our measure of vertex sets to be the number of vertices in S for a subset S of vertices:

$$h'(S) = \frac{|E(S, \bar{S})|}{\min |S|, |\bar{S}|}$$

and

$$h'_G = \inf_S h'(S).$$

2.2 The edge expansion of a graph

There are some fundamental relations between eigenvalues and the Cheeger constant. We first derive an upper bound for the eigenvalue λ_1 in terms of the Cheeger constant of a connected graph.

Lemma 2.1: $2h_G \geq \lambda_1$

Proof: We choose f based on an optimum edge cut C which achieves h_G and separates the graph G into two parts, A and B :

$$f(v) = \begin{cases} \frac{1}{\text{vol } A} & \text{if } v \text{ is in } A \\ -\frac{1}{\text{vol } B} & \text{if } v \text{ is in } B. \end{cases}$$

By substituting f into (1.2), we have the following:

$$\begin{aligned} \lambda_1 &\leq |C|(1/\text{vol } A + 1/\text{vol } B) \leq \\ &\leq \frac{2|C|}{\min(\text{vol } A, \text{vol } B)} = \\ &= 2h_G. \end{aligned}$$

□

Next we derive a lower bound for the eigenvalue λ_1 . This will give us the *Cheeger inequality*: $2h_G \geq \lambda_1 > \frac{h_G^2}{2}$.

Theorem 2.2: For a connected graph G , one has $\lambda_1 > \frac{h_G^2}{2}$.

Proof: We consider the harmonic eigenfunction f of \mathcal{L} with eigenvalue λ_1 . We order vertices of G according to f . That is, relabel the vertices so that $f(v_i) \leq f(v_{i+1})$, for $1 \leq i \leq n-1$. Without loss of generality, we may assume that

$$\sum_{f(v)<0} d_v \geq \sum_{f(u)\geq 0} d_u.$$

For each $i, 1 \leq i \leq |V|$, we consider the cut

$$C_i = \{\{v_j, v_k\} \in E(G) : 1 \leq j \leq i < k \leq n\}.$$

We define α by

$$\alpha = \min_{1 \leq i \leq n} \frac{|C_i|}{\min(\sum_{j \leq i} d_j, \sum_{j > i} d_j)}.$$

It is clear that $\alpha \geq h_G$. We consider the set V_+ of vertices v satisfying $f(v) \geq 0$ and the set E_+ of edges $\{u, v\}$ in G with either u or v in V_+ . We define

$$g(x) = \begin{cases} f(x) & \text{if } x \in V_+ \\ 0 & \text{otherwise.} \end{cases}$$

We now have

$$\begin{aligned} \lambda_1 &= \frac{\sum_{v \in V_+} f(v) \sum_{\{u,v\} \in E_+} (f(v) - f(u))}{\sum_{v \in V_+} f^2(v) d_v} > \\ &> \frac{\sum_{\{u,v\} \in E_+} (g(u) - g(v))^2}{\sum_{v \in V} g^2(v) d_v} = \\ &= \frac{\sum_{\{u,v\} \in E_+} (g(u) - g(v))^2 \sum_{\{u,v\} \in E_+} (g(u) + g(v))^2}{\sum_{v \in V} g^2(v) d_v \sum_{\{u,v\} \in E_+} (g(u) + g(v))^2} \geq \\ &\geq \frac{(\sum_{u \sim v} |g^2(u) - g^2(v)|)^2}{2(\sum_v g^2(v) d_v)^2} \geq \end{aligned}$$

$$\begin{aligned}
& \geq \frac{(\sum_i |g^2(v_i) - g^2(v_{i+1})| |C_i|)^2}{2(\sum_v g^2(v) d_v)^2} \geq \\
& \geq \frac{(\sum_i (g^2(v_i) - g^2(v_{i+1})) \alpha \sum_{j \leq i} d_j)^2}{2(\sum_v g^2(v) d_v)^2} \geq \\
& \geq \frac{\alpha^2}{2} \geq \frac{h_G^2}{2}.
\end{aligned}$$

□

The next Theorem will give an improved version of Theorem 2.2.

Theorem 2.3: *For a connected graph G , we always have $\lambda_1 > 1 - \sqrt{1 - h_G^2}$.*

Proof: From the proof of Theorem 2.2 we have

$$\begin{aligned}
\lambda_1 &= \frac{\sum_{v \in V_+} f(v) \sum_{u \sim v} (f(v) - f(u))}{\sum_{v \in V_+} f^2(v) d_v} > \\
&> \frac{\sum_{\{u,v\} \in E_+} (g(u) - g(v))^2}{\sum_{v \in V} g^2(v) d_v} = W.
\end{aligned}$$

Also we have

$$\begin{aligned}
W &= \frac{\sum_{\{u,v\} \in E_+} (g(u) - g(v))^2 \sum_{\{u,v\} \in E_+} (g(u) + g(v))^2}{\sum_{v \in V} g^2(v) d_v \sum_{\{u,v\} \in E_+} (g(u) + g(v))^2} \geq \\
&\geq \frac{(\sum_{u \sim v} |g^2(u) - g^2(v)|)^2}{(\sum_v g^2(v) d_v)(2 \sum_v g^2(v) d_v - W \sum_v g^2(v) d_v)} \geq \\
&\geq \frac{(\sum_i |g^2(v_i) - g^2(v_{i+1})| |C_i|)^2}{(2 - W)(\sum_v g^2(v))^2 d_v} \geq \\
&\geq \frac{(\sum_i (g^2(v_i) - g^2(v_{i+1})) \alpha \sum_{j \leq i} d_j)^2}{(2 - W)(\sum_v g^2(v))^2 d_v} \geq \\
&\geq \frac{\alpha^2}{2 - W}.
\end{aligned}$$

This implies that $W^2 - 2W + \alpha^2 \leq 0$. Therefore we have

$$\begin{aligned}\lambda_1 > W &\geq 1 - \sqrt{1 - \alpha^2} \geq \\ &\geq 1 - \sqrt{1 - h_G^2}.\end{aligned}$$

□

Corollary 2.4: *In a graph G with the eigenfunction f associated with λ_1 , we define, for each v , $C_v = \{\{u, u'\} \in E(G) : f(u) \leq f(v) < f(u')\}$ and*

$$\alpha = \min_v \frac{|C_v|}{\min\left(\sum_{\substack{u \\ f(u) \leq f(v)}} d_u, \sum_{\substack{u \\ f(u) > f(v)}} d_u\right)}. \text{ Then } \lambda_1 > 1 - \sqrt{1 - \alpha^2}.$$

One immediate consequence is an improvement on the range of λ_1 . For any connected (simple) graph G , we have $h_G \geq \frac{2}{\text{vol } G}$. Using Cheeger's inequality, we have $\lambda_1 > \frac{1}{2} \left(\frac{2}{\text{vol } G} \right)^2 \geq \frac{2}{n^4}$.

Chapter 3

Diameter and eigenvalues

3.1 The diameter of a graph

We define the length of a shortest path joining u and v in a graph G to be the distance between two vertices u and v , denoted by $d(u, v)$. The maximum distance over all pairs of vertices in G , denoted by $D(G)$, is called the diameter of G . The diameter is closely related to eigenvalues. This connection is based on the following observation:

Let M denote an $n \times n$ matrix with rows and columns indexed by the vertices of G . Suppose G satisfies the property that $M(u, v) = 0$ if u and v are not adjacent. Furthermore, suppose we can show that for some integer t , and some polynomial $p_t(x)$ of degree t , we have $p_t(M)(u, v) \neq 0$ for all u and v . Then we can conclude that the diameter $D(G)$ satisfies: $D(G) \leq t$.

Suppose we take M to be the sum of the adjacency matrix and the identity matrix and the polynomial $p_t(x)$ to be just $(1 + x)^t$. The following inequality for regular graphs which are not complete graphs can then be derived (which will be proved in Section 3.2):

$$D(G) \leq \left\lceil \frac{\log(n-1)}{\log(1/(1-\lambda))} \right\rceil. \quad (3.1)$$

Here, λ basically only depends on λ_1 . We can take $\lambda = \lambda_1$ if $1 - \lambda_1 \geq \lambda_{n-1} - 1$. The inequality (3.1) can be improved if we define $\lambda = 2\lambda_1/(\lambda_{n-1} + \lambda_1) \geq 2\lambda_1/(2 + \lambda_1)$, and we then have

$$D(G) \leq \left\lceil \frac{\log(n-1)}{\log \frac{\lambda_{n-1} + \lambda_1}{\lambda_{n-1} - \lambda_1}} \right\rceil. \quad (3.2)$$

The bound in (3.1) can be further improved by choosing p_t to be the Chebyshev polynomial of degree t . We can then replace the logarithmic function by \cosh^{-1} :

$$D(G) \leq \left\lceil \frac{\cosh^{-1}(n-1)}{\cosh^{-1} \frac{\lambda_{n-1} + \lambda_1}{\lambda_{n-1} - \lambda_1}} \right\rceil.$$

The diameter is the least integer t such that the matrix $M = I + A$ has the property that all entries of M^t are nonzero.

3.2 Eigenvalues and distances between two subsets

We define for two subsets X, Y of vertices in G , the distance $d(X, Y)$ between X and Y , as the minimum distance between a vertex in X and a vertex in Y . We have $d(X, Y) = \min\{d(x, y) : x \in X, y \in Y\}$. Let \bar{X} denote the complement of X in $V(G)$.

Theorem 3.1: *Suppose that G is not a complete graph. For $X, Y \subset V(G)$ and $X \neq \bar{Y}$, we have*

$$d(X, Y) \leq \left\lceil \frac{\log \sqrt{\frac{\text{vol } \bar{X} \text{ vol } \bar{Y}}{\text{vol } X \text{ vol } Y}}}{\log \frac{\lambda_{n-1} + \lambda_1}{\lambda_{n-1} - \lambda_1}} \right\rceil. \quad (3.3)$$

Proof: For $X \subset V(G)$, we define $\psi_X(x) = \begin{cases} 1 & \text{if } x \in X \\ 0 & \text{otherwise} \end{cases}$.

If we can show that for some integer t and some polynomial $p_t(z)$ of degree t , one has $\langle T^{1/2}\psi_Y, p_t(\mathcal{L})(T^{1/2}\psi_X) \rangle > 0$ then there is a path of length at most t joining a vertex in X to a vertex in Y . Therefore we have $d(X, Y) \leq t$.

Let a_i denote the "Fourier" coefficients of $T^{1/2}\psi_X$, i.e., $T^{1/2}\psi_X = \sum_{i=0}^{n-1} a_i \phi_i$,

where the ϕ_i 's are the orthogonal eigenfunctions of \mathcal{L} . In particular, we have $a_0 = \frac{\langle T^{1/2}\psi_X, T^{1/2}\mathbf{1} \rangle}{\langle T^{1/2}\mathbf{1}, T^{1/2}\mathbf{1} \rangle} = \frac{\text{vol } X}{\text{vol } G}$. Similarly, we write $T^{1/2}\psi_Y = \sum_{i=0}^{n-1} b_i \phi_i$.

Suppose we choose $p_t(z) = (1 - \frac{2z}{\lambda_1 + \lambda_{n-1}})^t$. Since G is not a complete graph, $\lambda_1 \neq \lambda_{n-1}$, and $|p_t(\lambda_i)| \leq (1 - \lambda)^t$ for all $i = 1, \dots, n-1$, where $\lambda = 2\lambda_1 / (\lambda_{n-1} + \lambda_1)$. Therefore we have

$$\begin{aligned} \langle T^{1/2}\psi_Y, p_t(\mathcal{L})(T^{1/2}\psi_X) \rangle &= a_0 b_0 + \sum_{i>0} p_t(\lambda_i) a_i b_i \geq \\ &\geq a_0 b_0 - (1 - \lambda)^t \sqrt{\sum_{i>0} a_i^2 \sum_{i>0} b_i^2} = \\ &= \frac{\text{vol } X \text{ vol } Y}{\text{vol } G} - (1 - \lambda)^t \frac{\sqrt{\text{vol } X \text{ vol } \bar{X} \text{ vol } Y \text{ vol } \bar{Y}}}{\text{vol } G}. \end{aligned}$$

By using the fact that

$$\sum_{i>0} a_i^2 = \|T^{1/2}\psi_X\|^2 - \frac{(\text{vol } X)^2}{\text{vol } G} = \frac{\text{vol } X \text{ vol } \bar{X}}{\text{vol } G}.$$

We note that in the above inequality, the equality holds if and only if $a_i = cb_i$ for some constant c for all i . This can only happen when $X = Y$ or $X = \bar{Y}$. Since the theorem obviously holds for $X = Y$ and we have the hypothesis that $X \neq \bar{Y}$,

we may assume that the inequality is strict. If we choose $t \geq \frac{\log \sqrt{\frac{\text{vol } \bar{X} \text{ vol } \bar{Y}}{\text{vol } X \text{ vol } Y}}}{\log \frac{1}{1-\lambda}}$ we have $\langle T^{1/2}\psi_Y, p_t(\mathcal{L})(T^{1/2}\psi_X) \rangle > 0$. \square

As an immediate consequence of Theorem 3.1, we have

Corollary 3.2: *Suppose G is a regular graph which is not a complete graph. Then*

$$D(G) \leq \left\lfloor \frac{\log(n-1)}{\log \frac{\lambda_{n-1} + \lambda_1}{\lambda_{n-1} - \lambda_1}} \right\rfloor.$$

To improve the inequality in (3.3) in some cases, we consider Chebyshev polynomials defined by:

$$T_0(z) = 1$$

$$T_1(z) = z$$

$$T_{t+1}(z) = 2zT_t(z) - T_{t-1}(z) \quad \text{for integer } t > 1.$$

Equivalently, we have $T_1(z) = \cosh(t \cosh^{-1}(z))$.

In place of $p_t(\mathcal{L})$, we will use $S_t(\mathcal{L})$, where $S_t(x) = \frac{T_t(\frac{\lambda_1 + \lambda_{n-1} - 2x}{\lambda_{n-1} - \lambda_1})}{T_t(\frac{\lambda_{n-1} + \lambda_1}{\lambda_{n-1} - \lambda_1})}$.

Then we have $\max_{x \in |\lambda_1, \lambda_{n-1}|} S_t(\lambda_1) \geq \frac{1}{T_t(\frac{\lambda_{n-1} + \lambda_1}{\lambda_{n-1} - \lambda_1})}$.

Suppose we take $t \geq \frac{\cosh^{-1} \sqrt{\frac{\text{vol } \bar{X} \text{ vol } \bar{Y}}{\text{vol } X \text{ vol } Y}}}{\cosh^{-1} \frac{\lambda_{n-1} + \lambda_1}{\lambda_{n-1} - \lambda_1}}$. Then we have

$$\langle T^{1/2} \psi_Y, S_t(\mathcal{L}) T^{1/2} \psi_X \rangle > 0.$$

Theorem 3.3: *Suppose G is not a complete graph. For $X, Y \subset V(G)$ and*

$$X \neq \bar{Y}, \text{ we have } d(X, Y) \leq \left\lfloor \frac{\cosh^{-1} \sqrt{\frac{\text{vol } \bar{X} \text{ vol } \bar{Y}}{\text{vol } X \text{ vol } Y}}}{\cosh^{-1} \frac{\lambda_{n-1} + \lambda_1}{\lambda_{n-1} - \lambda_1}} \right\rfloor.$$

For a subset $X \subset Y$, we define the s -boundary of X by

$$\delta_s X = \{y : y \notin X \text{ and } d(x, y) \leq s, \text{ for some } x \in X\}.$$

$\delta_1(x)$ is exactly the vertex boundary $\delta(x)$. If we choose $Y = V - \delta_s X$ in (3.3).

From the proof of Theorem 3.3, we have

$$0 = \langle T^{1/2} \psi_Y, (I - \mathcal{L})^t T^{1/2} \psi_X \rangle > \frac{\text{vol } X \text{ vol } Y}{\text{vol } G} - (1 - \lambda)^t \frac{\sqrt{\text{vol } X \text{ vol } \bar{X} \text{ vol } Y \text{ vol } \bar{Y}}}{\text{vol } G}.$$

This implies

$$(1 - \lambda)^{2t} \text{vol } \bar{X} \text{ vol } \bar{Y} \geq \text{vol } X \text{ vol } Y. \quad (3.4)$$

For the case of $t = 1$, we have the following:

Lemma 3.4: *For all $X \subseteq V(G)$, we have $\frac{\text{vol } \delta X}{\text{vol } X} \geq \frac{1 - (1 - \lambda)^2}{(1 - \lambda)^2 + \text{vol } X / \text{vol } \bar{X}}$, where $\lambda = 2\lambda_1 / (\lambda_{n-1} + \lambda_1)$.*

Proof: Lemma 3.4 clearly holds for complete graphs. Suppose G is not complete, and take $Y = \bar{X} - \delta X$ and $t = 1$. From the proof of Theorem 3.1, we

have

$$0 = \langle T^{1/2}\psi_Y, p_t(\mathcal{L})T^{1/2}\psi_X \rangle > \frac{\text{vol } X \text{ vol } Y}{\text{vol } G} - (1-\lambda) \frac{\sqrt{\text{vol } X \text{ vol } \bar{X} \text{ vol } Y \text{ vol } \bar{Y}}}{\text{vol } G}.$$

Thus $(1-\lambda)^2 \text{vol } \bar{X} \text{ vol } \bar{Y} > \text{vol } X \text{ vol } Y$. Since $\bar{Y} = X \cup \delta X$, this implies $(1-\lambda)^2(\text{vol } G - \text{vol } X)(\text{vol } X + \text{vol } \delta X) > \text{vol } X(\text{vol } G - \text{vol } X - \text{vol } \delta X)$.

After cancelation we obtain $\frac{\text{vol } \delta X}{\text{vol } X} \geq \frac{1 - (1-\lambda)^2}{(1-\lambda)^2 + \text{vol } X/\text{vol } \bar{X}}$. \square

Corollary 3.5: For $X \subseteq V(G)$ with $\text{vol } X \leq \text{vol } \bar{X}$, where G is not a complete graph, we have $\frac{\text{vol } \delta X}{\text{vol } X} \geq \lambda$, where $\lambda = 2\lambda_1/(\lambda_{n-1} + \lambda_1)$.

Proof: This follows from the fact that $\frac{\text{vol } \delta X}{\text{vol } X} \geq \frac{1 - (1-\lambda)^2}{1 + (1-\lambda)^2} \geq \lambda$ by using $\lambda \leq 1$. \square

For a general t , by a similar argument, we have

Lemma 3.6: For $X \subseteq V(G)$ and any integer $t > 0$, one has

$$\frac{\text{vol } \delta_t X}{\text{vol } X} \geq \frac{1 - (1-\lambda)^{2t}}{(1-\lambda)^{2t} + \text{vol } X/\text{vol } \bar{X}} \quad \text{where } \lambda = 2\lambda_1/(\lambda_{n-1} + \lambda_1).$$

Lemma 3.7: For any integer $t > 0$ and $X \subseteq V(G)$ with $\text{vol } X \leq \text{vol } \bar{X}$,

$$\text{we have } \frac{\text{vol } \delta_t X}{\text{vol } X} \geq \frac{1 - (1-\lambda)^{2t}}{1 + (1-\lambda)^{2t}} \quad \text{where } \lambda = 2\lambda_1/(\lambda_{n-1} + \lambda_1).$$

Suppose we consider: $N_s^* X = X \cup \delta_s X$, for $X \subseteq V(G)$.

As a consequence of Lemma 3.6, we get

Lemma 3.8: For $X \subseteq V(G)$ with $\text{vol } X \leq \text{vol } \bar{X}$ and any integer $t > 0$,

$$\frac{\text{vol } N_t^* X}{\text{vol } X} \geq \frac{1}{(1-\lambda)^{2t} \frac{\text{vol } \bar{X}}{\text{vol } G} + \frac{\text{vol } X}{\text{vol } G}}.$$

If $t = 1$ and G is a regular graph in Lemma 3.8 we have the basic inequality for establishing the vertex expansion properties of a graph.

Chapter 4

Paths and flows

4.1 Paths

Graph theory often deals with paths joining pairs of vertices. One example is the Hamiltonian path problem where we want to decide if a graph has a simple path containing every vertex of the graph. Some diameter and distance problems involve finding shortest paths. In many problems the sets of paths are either vertex disjoint or edge disjoint.

Consider a graph G with vertex set V and edge set E . (Two sets A and B are equinumerous if they have the same cardinality, i.e., if there exists a bijection $f : A \rightarrow B$. In sets, the category of all sets with functions as morphisms, an isomorphism between two sets is precisely a bijection, and two sets are equinumerous precisely if they are isomorphic). Let X and Y be two equinumerous subsets of vertices of G . In general, X and Y can be multisets and it is not necessary to require $X \cap Y = \emptyset$.

For $|X| = |Y| = m$, a *flow* F from X to Y consists of m paths in G joining the vertices in X to the vertices in Y . The *input* of the flow F is X and the *output* is Y . In a one-to-one fashion, paths in F join vertices of X to vertices of Y . It does not matter which vertex another vertex is "talking" to but the paths must be chosen so that no edge is overused. The paths might be required to be vertex disjoint or edge disjoint for instance.

4.2 Flows and Cheeger constants

There is a direct connection between the Cheeger constants and flow problems on graphs.

Lemma 4.1: *For a graph G on n vertices, suppose there is a set of $\binom{n}{2}$ paths joining all pairs of vertices such that each edge of G is contained in at most m*

paths. Then $h'_G = \sup_S \frac{|E(S, \bar{S})|}{\min(|S|, |\bar{S}|)} \geq \frac{n}{2m}$.

Proof: The proof follows from the fact that for any set $S \subseteq V$ with $|S| \leq |\bar{S}|$, we have $|E(S, \bar{S})| \cdot m \geq |S| \cdot |\bar{S}| \geq |S| \cdot \frac{n}{2}$ □

As an immediate consequence, we have the following:

Corollary 4.2: *For a k -regular graph G on n vertices, suppose there is a set P of $\binom{n}{2}$ paths joining all pairs of vertices such that each edge of G is contained in at most m paths in P . Then the Cheeger constant h_G satisfies*

$$h_G = \inf_S \frac{|E(S, \bar{S})|}{k \min(|S|, |\bar{S}|)} \geq \frac{n}{2mk}.$$

We can establish eigenvalue lower bounds for a regular graph, by using Cheeger's inequality and the above lower bound for the Cheeger constant from a flow. We can derive a better lower bound for λ_1 directly from a flow in a general graph. First a simple version for a regular graph.

Theorem 4.3: *For a k -regular graph G on n vertices, suppose there is a set P of $\binom{n}{2}$ paths joining all pairs of vertices such that each path in P has length at most l and each edge of G is contained in at most m paths in P . Then the eigenvalue λ_1 satisfies $\lambda_1 \geq \frac{n}{kml}$.*

Proof: Consider the harmonic eigenfunction $f : V(G) \rightarrow \mathbb{R}$ achieving λ_1 . Then,

$$\lambda_1 = \frac{n \sum_{\{x,y\} \in E(G)} (f(x) - f(y))^2}{k \sum_{x,y} (f(x) - f(y))^2}.$$

For $x, y \in V(G)$ and the path $P(x, y)$ joining x and y in G , we have

$$(f(x) - f(y))^2 \leq |P(x, y)| \sum_{e \in P(x, y)} f^2(e) \leq l \sum_{e \in P(x, y)} f^2(e), \text{ where}$$

$f^2(e) = (f(x) - f(y))^2$ for $e = \{x, y\}$, and $|P(x, y)|$ denotes the number of edges of G in $P(x, y)$. Hence

$$m \sum_{e \in E(G)} f^2(e) \geq \sum_{x,y} \sum_{e \in P(x,y)} f^2(e) \geq \frac{1}{l} \sum_{x,y} (f(x) - f(y))^2.$$

Therefore we have $\lambda_1 \geq \frac{n}{kml}$. □

This can be generalized for a general graph as follows:

Theorem 4.4: *For an undirected graph G , replace each edge $\{u, v\}$ by two directed edges (u, v) and (v, u) . Suppose there is a set P of $4e^2$ paths such that for each (ordered) pair of directed edges there is a directed path joining them. In addition, assume that each directed edge of G is contained in at most m directed paths in P . Then the Cheeger constant h_G satisfies $h_G = \frac{|E(S, \bar{S})|}{\min(\text{vol } S, \text{vol } \bar{S})} \geq \frac{\text{vol } G}{2m}$.*

Proof: For any $S \subseteq V(G)$, we have $m|E(S, \bar{S})| \geq \text{vol } S \text{ vol } \bar{S} \geq \frac{\text{vol } S \text{ vol } G}{2}$. □

Theorem 4.5: *For an undirected graph G , replace each edge $\{u, v\}$ by two directed edges (u, v) and (v, u) . Suppose there is a set P of $4e^2$ paths such that for each (ordered) pair of directed edges there is a directed path joining them, each of length at most l . In addition, assume that each directed edge of G is contained in at most m directed paths in P . Then the eigenvalue λ_1 satisfies $\lambda_1 \geq \frac{\text{vol } G}{ml}$.*

The proof is very similar to that of Theorem (4.3) and will be omitted.

Chapter 5

Cheeger constants and eigenvalues of symmetrical graphs

5.1 Cheeger constants of symmetrical graphs

For a graph G , an *automorphism* $f : V(G) \rightarrow V(G)$ is a one-to-one mapping which preserves edges, i.e, for $u, v \in V(G)$, we have $\{u, v\} \in E$ if and only if $\{f(u), f(v)\} \in E$.

The automorphism group of a graph, acts on the set of vertices of the graph. The action of a group G' on X is called *transitive* if for any two x, y in X there exists an g in G' such that $gx = y$.

A graph G is called *vertex-transitive* if its automorphism group $Aut(G)$ acts transitively on the vertex set $V(G)$, i.e, for any two vertices u and v there is an automorphism $f \in Aut(G)$ such that $f(u) = v$.

A graph G is called *edge-transitive* if, for any two edges $\{x, y\}, \{z, w\} \in E(G)$, there is an automorphism f such that $\{f(x), f(y)\}, \{z, w\}$.

Theorem 5.1: *Suppose Γ is a finite edge-transitive graph of diameter D . Then the Cheeger constant h_Γ satisfies $h_\Gamma \geq \frac{1}{2D}$.*

Proof: Let S denote a subset of vertices such that $|S| \leq \frac{n}{2}$ where $n = |V(\Gamma)|$. We consider a random (ordered) pair of vertices (x, y) , uniformly chosen over $V(\Gamma) \times V(\Gamma)$. Now we choose randomly a shortest path P between x and y (uniformly chosen over all possible shortest paths). Since Γ is edge-transitive the probability that P goes through a given edge is at most $\frac{2D}{\text{vol } \Gamma}$. A path between a vertex from S and a vertex from \bar{S} must contain an edge in $E(S, \bar{S})$. Therefore we have $\frac{2|E(S, \bar{S})| \cdot D}{\text{vol } \Gamma} \geq \text{Prob}(x \in S, y \in \bar{S} \text{ or } x \in \bar{S}, y \in S)$.

This implies

$$\begin{aligned} |E(S, \bar{S})| &\geq \frac{|S||\bar{S}|\text{vol } \Gamma}{Dn^2}, \\ |E(S, \bar{S})| &\geq \frac{|\bar{S}|}{Dn} \geq \\ &\geq \frac{1}{2D}. \end{aligned}$$

Therefore $h_\Gamma \geq \frac{1}{2D}$. □

Theorem 5.2: *Suppose Γ is a finite vertex-transitive graph of diameter D and degree k . Then the Cheeger constant h_Γ satisfies $h_\Gamma \geq \frac{1}{2kD}$.*

Proof: The automorphism group defines an equivalence relation on the edges of Γ . Two edges e_1, e_2 are equivalent if and only if there is an automorphism π mapping e_1 to e_2 . We can then consider equivalence classes of edges, denoted by E_1, \dots, E_s . We define the index of Γ to be $\text{index } \Gamma = \min_i \frac{\text{vol } \Gamma}{2|E_i|}$ where E_i denotes the i -th equivalence class of edges. Clearly, we have $1 \leq \text{index } \Gamma \leq k$. In particular, when Γ is edge-transitive, we have $\text{index } \Gamma = 1$.

Since Γ is vertex-transitive, each equivalence class contains at least $\frac{n}{2}$ edges. Let p_i denote the probability that a pair of vertices is an edge in the i -th equivalence class E_i . Since all edges in the same equivalence class have the same probability, we have, for each i , $p_i \leq \frac{1}{|E_i|} \leq \frac{2 \text{index } \Gamma}{\text{vol } \Gamma}$. For a subset S of the vertex set with $\text{vol } S \leq \text{vol } \bar{S}$ and for a pair of vertices x, y in $\Gamma(G)$, the probability of having one of x, y in S and the other in \bar{S} is the same as the probability that $P(x, y)$ contains an edge in $E(S, \bar{S})$. Therefore we have

$$\text{Prob}(x \in S, y \in \bar{S} \text{ or } x \in \bar{S}, y \in S) \leq |E(S, \bar{S})| D \max_i p_i \leq |E(S, \bar{S})| D \frac{2 \text{index } \Gamma}{\text{vol } \Gamma}.$$

Since $\text{Prob}(x \in S, y \in \bar{S} \text{ or } x \in \bar{S}, y \in S) = \frac{2|S||\bar{S}|}{n^2}$ we have

$$\frac{|E(S, \bar{S})|}{\text{vol } S} \geq \frac{1}{2D \text{index } \Gamma} \geq \frac{1}{2kD}.$$

□

The above proof gives the following slightly stronger result:

Theorem 5.3: *Suppose Γ is a finite vertex-transitive graph of diameter D . Then $h_\Gamma \geq \frac{1}{2D \text{index } \Gamma}$.*

5.2 Eigenvalues of symmetrical graphs

We here derive some stronger lower bounds, for eigenvalues of edge-transitive and vertex-transitive graphs, than the bounds, for general graphs, we get using Cheeger inequalities.

Theorem 5.4: *For an edge-transitive graph Γ with diameter D and degree*

k , we have $\lambda_1 \geq \frac{1}{D^2}$.

Theorem 5.5: For a vertex-transitive graph Γ with diameter D , we have $\lambda_1 \geq \frac{1}{kD^2}$.

The above two theorems are special cases of the following theorem:

Theorem 5.6: For a vertex-transitive graph Γ with diameter D , we have $\lambda_1 \geq \frac{1}{D^2 \text{index } \Gamma}$ where $\text{index } \Gamma = \min \frac{\text{vol } \Gamma}{2|E_i|}$, and where E_i , denotes the i -th equivalence class of edges under $\text{Aut}(\Gamma)$.

Proof: We consider $f : V(\Gamma) \rightarrow \mathbb{R}$ and we use the (equivalent) eigenvalue definition (1.5) in Chapter 1:

$$\lambda_1 = \min_f \frac{n \sum_{x \sim y} (f(x) - f(y))^2}{k \sum_x \sum_y (f(x) - f(y))^2}.$$

For each edge $e = \{x, y\}$, we define $f(e) = |f(x) - f(y)|$. We then have

$$\lambda_1 = \min_f \frac{n \sum_{e \in E} f^2(e)}{k \sum_x \sum_y (f(x) - f(y))^2}.$$

Let E_i denotes the i -th equivalence class of edges under $\text{Aut}(\Gamma)$. For a fixed vertex x_0 , we choose a fixed set of shortest paths $P_{x_0, y}$ to all y in Γ . We can now use the automorphism group to define, for each vertex $x \in V(\Gamma)$ and an automorphism π with $\pi(x_0) = x$, a set of paths $P(x) = \{\pi(P_{x_0, y})\}$. Clearly, each path in $P(x)$ has length at most D . For each edge e , we consider the number N_e of occurrences of e in paths in $P(x)$ ranging over all x .

Two edges in the same equivalence class have the same value for N_e . The total number of edges in all paths in $P(x)$ for all x is at most $n^2 D$. For each i and $e \in E_i$, we have $N_e \leq \frac{n^2 D}{2|E_i|} \leq \frac{n^2 D}{2 \min_i |E_i|} = \frac{nD \text{index } \Gamma}{\text{vol } \Gamma} = \frac{D \text{index } \Gamma}{k}$.

Now we consider, for a harmonic eigenfunction f achieving λ_1 ,

$$\begin{aligned} \sum_x \sum_y (f(x) - f(y))^2 &= \sum_x \sum_y \left(\sum_{e \in P(x, y)} f(e) \right)^2 \leq \\ &\leq \sum_x \sum_y D \sum_{e \in P(x, y)} f^2(e) \leq \\ &\leq \sum_{e \in E} f^2(e) D N_e \leq \\ &\leq \sum_{e \in E} f^2(e) D \frac{D \text{index } \Gamma}{k}. \end{aligned}$$

Therefore we have

$$\lambda_1 = \frac{n \sum_{e \in E} f^2(e)}{k \sum_x \sum_y (f(x) - f(y))^2} \geq \frac{1}{D^2 \text{ index } \Gamma}.$$

□

Chapter 6

Dirichlet eigenvalues and a matrix-tree theorem

6.1 Dirichlet eigenvalues

The Laplacian \mathcal{L} acts on functions with the *Dirichlet boundary condition*. We consider, for a subset S of the vertices of G , the space of functions $\{f : S \cup \delta S \rightarrow \mathbb{R}\}$ which satisfy the Dirichlet condition

$$f(x) = 0 \quad (6.1)$$

for any vertex x in the vertex boundary δS of S .

In a graph G with vertex set $V = V(G)$ and edge set $E = E(G)$, let S denote a subset of V and assume that the vertex boundary δS is nonempty. $f \in D^*$ denotes that f satisfies the Dirichlet boundary condition in (6.1). That is: $f(x) = 0$ for $x \in \delta S$. The Dirichlet eigenvalues of an induced subgraph on S are defined as follows:

$$\begin{aligned} \lambda_1^{(D)} &= \inf_{\substack{f \neq 0 \\ f \in D^*}} \frac{\sum_{\{x,y\} \in S^*} (f(x) - f(y))^2}{\sum_{x \in S} f^2(x) d_x} = & (6.2) \\ &= \inf_{\substack{g \neq 0 \\ g \in D^*}} \frac{\sum_{\{x,y\} \in S^*} \left(\frac{g(x)}{\sqrt{d_x}} - \frac{g(y)}{\sqrt{d_y}} \right)^2}{\sum_{x \in S} g(x)^2} = \\ &= \inf_{\substack{g \neq 0 \\ g \in D^*}} \frac{\langle g, \mathcal{L}g \rangle}{\langle g, g \rangle}. \end{aligned}$$

In general, we define the i -th Dirichlet eigenvalue λ_i to be

$$\lambda_1^{(D)} = \inf_{f \neq 0} \sup_{f' \in C_{i-1}} \frac{\sum_{\{x,y\} \in S^*} (f(x) - f(y))^2}{\sum_{x \in S} (f(x) - f'(y))^2 d_x}$$

where C_i is the subspace spanned by eigenfunctions ϕ_j achieving λ_j , for $1 \leq j \leq i$. We put $\lambda_1^{(D)} = \lambda_S^{(D)}$. For a connected induced subgraph S of a graph G with $\partial S \neq \emptyset$, we have $0 < \lambda_1^{(D)} \leq \frac{|\partial S|}{\text{vol } S} \leq 1$ and $0 < \lambda_i^{(D)} \leq 2$ for $1 \leq i \leq |S|$.

Lemma 6.1: *For an induced subgraph S , let g denote an eigenfunction of \mathcal{L} with Dirichlet eigenvalue λ , i.e., $g : S \rightarrow \mathbb{R}$ satisfies (6.2) and the Dirichlet boundary condition $g(x) = 0$ for $x \in \delta S$. Then g satisfies*

(1) : for $x \in S$,

$$\mathcal{L}g(x) = \frac{1}{\sqrt{d_x}} \sum_{\substack{y \\ \{x,y\} \in S^*}} \left(\frac{g(x)}{\sqrt{d_x}} - \frac{g(y)}{\sqrt{d_y}} \right) = \lambda g(x)$$

(2) : for any function $h : V \rightarrow \mathbb{R}$,

$$\sum_{x \in S} h(x) \mathcal{L}g(x) = \sum_{\{x,y\} \in S^*} \left(\frac{h(x)}{\sqrt{d_x}} - \frac{h(y)}{\sqrt{d_y}} \right) \cdot \left(\frac{g(x)}{\sqrt{d_x}} - \frac{g(y)}{\sqrt{d_y}} \right)$$

The proof of (1) follows from the variational principles. To see (2), we note that

$$\sum_{x \in S} h(x) \mathcal{L}g(x) - \sum_{\{x,y\} \in S^*} \left(\frac{h(x)}{\sqrt{d_x}} - \frac{h(y)}{\sqrt{d_y}} \right) \cdot \left(\frac{g(x)}{\sqrt{d_x}} - \frac{g(y)}{\sqrt{d_y}} \right) = \sum_{x \in \delta S} \frac{g(x)}{\sqrt{d_x}} \left(\frac{h(x)}{\sqrt{d_x}} - \frac{h(y)}{\sqrt{d_y}} \right) = 0.$$

As a consequence of Lemma 6.1, for functions $f : S \rightarrow \mathbb{R}$ under the assumption that $f(y) = 0$ for $y \in \delta S$, we have, for all $x \in S$, the equality $\mathcal{L}f(x) = \mathcal{L}_S f(x)$ where \mathcal{L}_S is the submatrix of \mathcal{L} restricted to columns and rows indexed by vertices in S . We note that since $\delta S = \emptyset$, \mathcal{L}_S is nonsingular. All eigenvalues of \mathcal{L}_S are positive. Hence the Dirichlet eigenvalues of the induced subgraph on S are just the eigenvalues of \mathcal{L}_S and the determinant of \mathcal{L}_S can be

expressed as: $\det \mathcal{L}_S = \prod_{i=1}^{|S|} \lambda_i^{(D)}$.

6.2 A matrix-tree theorem and Dirichlet eigenvalues

The matrix-tree theorem states that the determinant of any cofactor of the combinatorial Laplacian is equal to number of spanning trees in a graph. We consider a generalization of the matrix-tree theorem for induced subgraphs of a graph. For an induced subgraph S with nonempty boundary in a graph G , we define a rooted spanning forest of S to be any subgraph F satisfying:

- (1) F is an acyclic subgraph of G
- (2) F has vertex set $S \cup \delta S$
- (3) Each connected component of F contains exactly one vertex in δS

Our next Theorem relates the product of the Dirichlet eigenvalues of S to the enumeration of rooted spanning forests of S .

Theorem 6.2: For an induced subgraph S in a graph G with $\delta \neq \emptyset$, the number of rooted spanning forests of S is $\prod_{x \in S} d_x \prod_{i=1}^{|S|} \lambda_i$ where $\lambda_i, 1 \leq i \leq |S|$, are the Dirichlet eigenvalues of the Laplacian of S in G .

Proof: We consider the incidence matrix B with rows indexed by vertices in S and columns indexed by edges in S^* defined as follows:

$$B(x, e) = \begin{cases} \frac{1}{\sqrt{d_x}} & \text{if } e = \{x, y\}, x < y \\ -\frac{1}{\sqrt{d_x}} & \text{if } e = \{x, y\}, x > y \\ 0 & \text{otherwise} \end{cases}$$

we have $\mathcal{L} = BB^*$ where B^* denotes the transpose of B . Then

$\prod_{i=1}^{|S|} \lambda_i = \det \mathcal{L} = \det BB^* = \sum_X \det B_X \det B_X^*$ where X ranges over all possible choices of $s - 1$ edges and B_X denotes the square submatrix of B whose $s - 1$ columns correspond to the edges in X .

Claim 1: If the subgraph with vertex set $S \cup \delta S$ and edge set X contains a cycle, then $\det B_X = 0$.

The proof follows from the fact that the columns restricted to those indexed by the cycle are dependent.

Claim 2: If the subgraph formed by edge set X contains a connected component having two vertices in δS , then $\det B_X = 0$.

Proof: Let Y denote a connected component of the subgraph formed by X . If Y contains more than one vertex in δS , then Y has no more than $|E(Y)| - 1$ vertices in S . The submatrix formed by the columns corresponding to the edges in Y has rank at most $|E(Y)| - 1$. Consequently, $\det B_X = 0$.

Claim 3: If the subgraph formed by X is a rooted forest of S , then

$$|\det B_X| = \frac{1}{\prod_{x \in S} \sqrt{d_x}}.$$

Proof: From Claims 1 and 2, we know that edges of X form a forest and each connected component contains exactly one vertex in δS . There is a column indexes by an edge with only one nonzero entry, say (x_1, e_1) with $x_1 \in S$.

Therefore, $|\det B_x| = \frac{1}{\sqrt{d_{x_1}}} |\det B_{x_1}^{(1)}|$ where $B_{x_1}^{(1)}$ denotes the submatrix with

rows indexed by $S - \{x_1\}$ and columns indexed by $X - \{e\}$. By removing one edge and one vertex at a time, we eventually obtain $|\det B_x| = \frac{1}{\prod_{x \in S} \sqrt{d_x}}$.

Combining Claims 1-3, we have

$$\prod_{i=1}^{|S|} \lambda_i = \det \mathcal{L} = \sum_X \det B_X \det B_X^* = \frac{1}{\prod_{x \in S} d_x} |\{\text{rooted spanning forests of } S\}|.$$

This completes the proof of Theorem 6.2. □

If we, for a graph G , apply Theorem 6.2 to an induced subgraph H on $V(G) - \{v\}$ for some vertex v in G , the rooted spanning forest correspond in a one-to-one fashion to all trees in G . So the usual matrix-tree theorem can be viewed as a special case of Theorem 6.2.

Conclusion

On our journey towards the matrix-tree theorem we have encountered some key elements, such as the Laplacian of a graph and how to receive the eigenvalues of the Laplacian. The set of eigenvalues we referred to as the spectrum of the graph. Then we moved on to the Cheeger constant and defined edge and vertex boundary to answer some problems, and looked at the relationship between eigenvalues and the Cheeger constant.

In chapter three we came across the diameter of a graph and distances between subsets of vertices, and got aware of the bond connecting these and eigenvalues. After that we returned to the Cheeger constant and its relation with paths and flows and then in the following chapter we spoke about Cheeger constants and eigenvalues of symmetrical graphs.

Next it was time for the Dirichlet boundary condition and Dirichlet eigenvalues to make way for the matrix-tree theorem.

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