CHAPTER 3

Diameters and eigenvalues

3.1. The diameter of a graph

In a graph G, the distance between two vertices u and v, denoted by $d(u,v)$, is defined to be the length of a shortest path joining u and v in G. (It is possible to define the distance by various more general measures.) The diameter of G, denoted by $D(G)$, is the maximum distance over all pairs of vertices in G. The diameter is one of the key invariants in a graph which is not only of theoretical interest but also has a wide range of applications. When graphs are used as models for communication networks, the diameter corresponds to the delays in passing messages through the network, and therefore plays an important role in performance analysis and cost optimization.

Although the diameter is a combinatorial invariant, it is closely related to eigenvalues. This connection is based on the following simple 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 $(1+x)^t$. The following inequality for regular graphs which are not complete graphs can then be derived (which will be proved in Section 3.2 as a corollary to Theorem 3.1; also see [**59**]):

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

Here, λ basically only depends on λ_1. For example, we can take $\lambda = \lambda_1$ if $1 - \lambda_1 \geq \lambda_{n-1} - 1$. In general, we can slightly improve (3.1) by using the same "spectrum shifting" trick as in Section 1.5 (see Section 3.2). Namely, we define $\lambda = 2\lambda_1/(\lambda_{n-1} + \lambda_1) \geq 2\lambda_1/(2+\lambda_1)$, and we then have

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

We note that for some graphs the above bound gives a pretty good upper bound for the diameter. For example, for k-regular Ramanujan graphs (defined later in 6.3.6), we have $1-\lambda_1 = \lambda_{n-1}-1 = 1/(2\sqrt{k-1})$ so we get $D \leq \log(n-1)/(2\log(k-1))$ which is within a factor of 2 of the best possible bound.

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 $\cosh^{-1}$ (see [**65**] and Theorem 3.3):

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

The above inequalities can be generalized in several directions. Instead of considering distances between two vertices, we can relate the eigenvalue λ_1 to distances between two subsets of vertices (see Section 3.2). Furthermore, for any $k \geq 1$, we can relate the eigenvalue λ_k to distances among $k+1$ distinct subsets of vertices (see Section 3.3).

We will derive several versions of the diameter-eigenvalue inequalities. From these inequalities, we can deduce a number of isoperimetric inequalities which are closely related to expander graphs which will also be discussed in Chapter 6.

It is worth mentioning that the above discrete methods for bounding eigenvalues can be used to derive new eigenvalue upper bounds for compact smooth Riemannian manifolds [**78, 79**]. This will be discussed in the last section of this chapter.

In contrast to many other more complicated graph invariants, the diameter is easy to compute. 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. This can be determined by using $O(\log n)$ iterations of matrix multiplication. Using the current best known bound $\mathcal{M}(n)$ for matrix multiplication where

$$\mathcal{M}(n) = O(n^{2.376})$$

this diameter algorithm requires at most $O(\mathcal{M}(n)\log n)$ steps. The problem of determining distances of all pairs of vertices for an undirected graph can also be done in $O(\mathcal{M}(n)\log n)$ time. Seidel [**229**] gave a simple recursive algorithm by reducing this problem for a graph G to a graph G' in which $u \sim v$ if $d(u,v) \leq 2$. (For directed graphs, an $O(\sqrt{\mathcal{M}(n)n^3})$ algorithm can be found in [**10**].)

Another related problem is to find shortest paths between all pairs of vertices, which can be easily done in $O(n^3)$ steps (in fact $O(nm)$ is enough for a graph on n vertices and m edges). Apparently, we cannot compute all shortest paths explicitly in $o(n^3)$ time since some graphs can have cn^2 pairs of vertices having shortest paths of length at least $c'n$ each. However, we can compute a data structure that allows all shortest paths be constructed in time proportional to their lengths. For example, a matrix has its (u,v)-entry to be a neighbor of u in a shortest path connecting u and v. Seidel gave a randomized algorithm [**229**] to compute such a matrix in expected time $O(\mathcal{M}(n)\log n)$.

3.2. Eigenvalues and distances between two subsets

For two subsets X, Y of vertices in G, the distance between X and Y, denoted by $d(X, Y)$, is the minimum distance between a vertex in X and a vertex in Y, i.e.,

$$d(X, Y) = \min\{d(x, y) : x \in X, y \in Y\}.$$

Let $\bar{X}$ denote the complement of X in $V(G)$.

THEOREM 3.1. *In a graph G, for $X, Y \subset V(G)$ with distance at least 2, we have*

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

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,

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

then there is a path of length at most t joining a vertex in X to a vertex in Y. Therefore we have $d(X, Y) \le t$.

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 orthogonal eigenfunctions of $\mathcal{L}$. In particular, we have

$$a_0 = \frac{\langle T^{1/2}\psi_X, T^{1/2}\mathbf{1}\rangle}{\sqrt{\mathrm{vol}\ G}} = \frac{\mathrm{vol}\ X}{\sqrt{\mathrm{vol}\ G}}.$$

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, $\lambda_1 \ne \lambda_{n-1}$, and

$$|p_t(\lambda_i)| \le (1-\lambda)^t$$

for all $i = 1, \ldots, n-1$, where $\lambda = 2\lambda_1/(\lambda_{n-1}+\lambda_1)$. Therefore, we have

$$\begin{aligned} \langle T^{1/2}\psi_Y, p_t(\mathcal{L})(T^{1/2}\psi_X)\rangle &= a_0b_0 + \sum_{i>0} p_t(\lambda_i)a_ib_i \\ &\ge a_0b_0 - (1-\lambda)^t\sqrt{\sum_{i>0} a_i^2 \sum_{i>0} b_i^2} \\ &= \frac{\mathrm{vol}\ X\,\mathrm{vol}\ Y}{\mathrm{vol}\ G} - (1-\lambda)^t\frac{\sqrt{\mathrm{vol}\ X\,\mathrm{vol}\ \bar{X}\,\mathrm{vol}\ Y\,\mathrm{vol}\ \bar{Y}}}{\mathrm{vol}\ G} \qquad (3.4) \end{aligned}$$

by using the fact that

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

If the inequality (3.4) is strict, we can choose

$$t \geq \frac{\log \sqrt{\frac{\text{vol } \bar{X} \text{ vol } \bar{Y}}{\text{vol } X \text{ vol } Y}}}{\log \frac{1}{1-\lambda}}$$

and we have

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

Therefore $d(X,Y) \leq t$.

Suppose that the equality in (3.4) holds. Then the equality in Cauchy-Schwarz inequality implies that $|a_i| = |cb_i|$ for some c and $i > 0$. This implies $c^2 = (\text{vol}Y - b_0^2)/(\text{vol}X - a_0^2) = b_0^2/a_0^2$. Without loss of generality, we assume $c = b_0/a_0$. Furthermore, the equality $a_i b_i p_i(\lambda_i) = -|a_i b_i||p_i(\lambda_i)| = -|a_i b_i|(1-\lambda)^t$ implies that there is an integer k, $1 \leq k < n-1$ such that $\lambda_i = \lambda_1$ and $a_j = -cb_j$ for $1 \leq i \leq k$; and for $j > k$, $a_j = cb_j$ and $\lambda_i = \lambda_{n-1}$. For this very special case, we use an argument by Kirkland [**176**]. Since $\langle T^{1/2}\psi_X, \mathcal{L}T^{1/2}\psi_Y\rangle = 0$, we have $\sum_{i=1}^k a_i = \lambda_{n-1}/\lambda_1 \sum_{j>k} a_j^2$. For $t \geq 2$, we consider

$$\begin{aligned}\langle T^{1/2}\psi_X, \mathcal{L}^t T^{1/2}\psi_Y\rangle &\geq c\left(-\lambda_1^t \sum_{i=1}^k a_i^2 + \lambda_{n-1}^t \sum_{j>k} a_j^2\right) \\ &\geq c(-\lambda_1^{t-1}\lambda_{n-1} + \lambda_{n-1}^t)\sum_{j>k} a_j^2 \\ &> 0.\end{aligned}$$

This again implies $d(X,Y) \leq t$. This completes the proof of Theorem 3.3. □

As an immediate consequence of Theorem 3.3, we have

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

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

To improve the inequality in Theorem 3.3 in some cases, we consider Chebyshev polynomials:

$$\begin{aligned}T_0(z) &= 1, \\ T_1(z) &= z, \\ T_{t+1}(z) &= 2zT_t(z) - T_{t-1}(z), \quad \text{for integer } t > 1.\end{aligned}$$

Equivalently, we have

$$T_t(z) = \cosh(t \cosh^{-1}(z)).$$

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

$$\max_{x\in[\lambda_1,\lambda_{n-1}]} S_t(x) \geq \frac{1}{T_t(\frac{\lambda_{n-1}+\lambda_1}{\lambda_{n-1}-\lambda_1})}.$$

Suppose we take

$$t \geq \frac{\cosh^{-1}\sqrt{\frac{\mathrm{vol}\,\bar{X}\,\mathrm{vol}\,\bar{Y}}{\mathrm{vol}\,X\,\mathrm{vol}\,Y}}}{\cosh^{-1}\frac{\lambda_{n-1}+\lambda_1}{\lambda_{n-1}-\lambda_1}}.$$

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 $X \neq \bar{Y}$, we have*

$$d(X,Y) \leq \left\lceil \frac{\cosh^{-1}\sqrt{\frac{\mathrm{vol}\bar{X}\mathrm{vol}\bar{Y}}{\mathrm{vol}X\,\mathrm{vol}Y}}}{\cosh^{-1}\frac{\lambda_{n-1}+\lambda_1}{\lambda_{n-1}-\lambda_1}} \right\rceil.$$

As an immediate application of Theorem 3.3, we can derive a number of isoperimetric inequalities. For a subset $X \subset V$, we define the s-boundary of X by

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

Clearly, $\delta_1(x)$ is exactly the vertex boundary $\delta(x)$. Suppose we choose $Y = V - \delta_s X$ in (3.3). From the proof of Theorem 3.1, we have

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

This implies

$$(1-\lambda)^{2t}\mathrm{vol}\,\bar{X}\mathrm{vol}\,\bar{Y} \geq \mathrm{vol}\,X\;\mathrm{vol}\,Y. \tag{3.5}$$

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

Lemma 3.4. *For all $X \subseteq V(G)$, we have*

$$\frac{\mathrm{vol}\,\delta X}{\mathrm{vol}\,X} \geq \frac{1-(1-\lambda)^2}{(1-\lambda)^2 + \mathrm{vol}X/\mathrm{vol}\bar{X}}$$

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

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

Thus

$$(1-\lambda)^2\mathrm{vol}\,\bar{X}\;\mathrm{vol}\,\bar{Y} > \mathrm{vol}\,X\;\mathrm{vol}\,Y.$$

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 cancellation, we obtain

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

□

COROLLARY 3.5. *For* $X \subseteq V(G)$ *with* vol $X \leq$ 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 $\lambda \leq 1$. □

For general t, by a similar argument, we have

LEMMA 3.6. *For* $X \subseteq V(G)$ *and any integer* $t > 0$,

$$\frac{\text{vol } \delta_t X}{\text{vol } X} \geq \frac{1-(1-\lambda)^{2t}}{(1-\lambda)^{2t} + \text{vol}X/\text{vol}\bar{X}}$$

where $\lambda = 2\lambda_1/(\lambda_{n-1} + \lambda_1)$.

LEMMA 3.7. *For an integer* $t > 0$ *and* $X \subseteq V(G)$ *with* vol $X \leq$ vol $\bar{X}$, *we have*

$$\frac{\text{vol } \delta_t X}{\text{vol } X} \geq \frac{1-(1-\lambda)^{2t}}{1+(1-\lambda)^{2t}}$$

where $\lambda = 2\lambda_1/(\lambda_{n-1} + \lambda_1)$.

Suppose we consider, for $X \subseteq V(G)$,

$$N_s^* X = X \cup \delta_s X.$$

As a consequence of Lemma 3.6, we have

LEMMA 3.8. *For* $X \subseteq V(G)$ *with* vol $X \leq$ vol $\bar{X}$ *and any integer* $t > 0$,

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

We remark that the special case of Lemma 3.8 for a regular graph and $t = 1$ was first proved by Tanner [**240**] (also see [**9**]). This is the basic inequality for establishing the vertex expansion properties of a graph. We will return to this inequality in Chapter 6.

3.3. Eigenvalues and distances among many subsets

To generalize Theorem 3.1 to distances among k subsets of the vertices, we need the following geometric lemma [**78**].

LEMMA 3.9. *Let $x_1, x_2, \dots, x_{d+2}$ denote $d+2$ arbitrary vectors in d-dimensional Euclidean space. Then there are two of them, say, v_i, v_j ($i \neq j$) such that $\langle v_i, v_j\rangle \geq 0$.*

PROOF. We will prove this by induction. First, it is clearly true when $d = 1$. Assume that it is true for $(d-1)$-dimensional Euclidean space for some $d > 1$. Suppose that each pair of the given vectors has a negative scalar product. Let P be a hyperplane orthogonal to x_{d+2} and let x'_i be the projection of x_i on P for $i = 1, 2, \dots, d+1$. We claim that $\langle x'_i, x'_j\rangle < 0$ provided $i \neq j$. Since $\langle x_i, x_{d+2}\rangle < 0$, for $i \leq d+1$, all vectors x_i lie in the same half-space with respect to P, which implies that each of them can be represented in the form

$$x_i = x'_i + a_i e$$

where $a_i > 0$ and e is a unit vector orthogonal to P, and directed to the same half-space as all the x_i. Then we have

$$0 > \langle x_i, x_j\rangle = \langle x'_i - a_i e, x'_j - a_j e\rangle = \langle x'_i, x'_j\rangle + a_i a_j$$

which implies $\langle x'_i, x'_j\rangle < 0$. On the other hand, by the induction hypothesis, out of $d+1$ vectors $x'_i, i = 1, 2, \dots, d+1$ in the $(d-1)$-dimensional space P, there are two vectors with non-negative scalar product. This is a contradiction and the lemma is proved. $\square$

THEOREM 3.10. *Suppose G is not a complete graph. For $X_i \subset V(G), i = 0, 1, \dots, k$, we have*

$$\min_{i \neq j} d(X_i, X_j) \leq \max_{i \neq j} \left\lceil \frac{\log \sqrt{\frac{\mathrm{vol}\bar{X}_i \ \mathrm{vol}\bar{X}_j}{\mathrm{vol}X_i \ \mathrm{vol}X_j}}}{\log \frac{1}{1-\lambda_k}} \right\rceil$$

if $1 - \lambda_k \geq \lambda_{n-1} - 1$, and $X_i \neq \bar{X}_j$ for $i = 0, 1, \dots, k$.

PROOF. Let X and Y denote two distinct subsets among the X_i's. Using the notation as in Theorem 3.1, we consider

$$\langle T^{1/2}\psi_Y, (I-\mathcal{L})^t T^{1/2}\psi_X\rangle \quad \geq \quad a_0 b_0 + \sum_{i=1}^{k-1} (1-\lambda_i)^t a_i b_i - \sum_{i \geq k} (1-\lambda_k)^t |a_i b_i|.$$

For each $X_i, i = 0, 1, \dots, k$, we consider the vector consisting of the Fourier coefficients in the eigenfunction expansion of X_i. Suppose we define a scalar product for two such vectors $(a_1, \dots, a_{k-1})$ and $(b_1, \dots, b_{k-1})$ by

$$\sum_{i=1}^{k-1} (1-\lambda_i)^t a_i b_i.$$

From Lemma 3.9, we know that we can choose two of the subsets, say, X and Y with their associated vectors satisfying

$$\sum_{i=1}^{k-1}(1-\lambda_i)^t a_i b_i \geq 0.$$

Therefore, we have

$$\langle T^{1/2}\psi_Y, (I-\mathcal{L})^t T^{1/2}\psi_X\rangle \quad > \quad \frac{\mathrm{vol}X\ \mathrm{vol}Y}{\mathrm{vol}\ G} - (1-\lambda_k)^t \frac{\sqrt{\mathrm{vol}X\ \mathrm{vol}\bar{X}\ \mathrm{vol}Y\ \mathrm{vol}\bar{Y}}}{\mathrm{vol}\ G}$$

and Theorem 3.10 is proved. □

We note that the condition $1-\lambda_k \geq \lambda_{n-1}-1$ can be eliminated by modifying λ_k as in the proof of Theorem 3.1:

THEOREM 3.11. *For $X_i \subset V(G), i = 0, 1, \ldots, k$, we have*

$$\min_{i\neq j} d(X_i, X_j) \leq \max_{i\neq j} \left\lceil \frac{\log \sqrt{\frac{\mathrm{vol}\bar{X}_i\ \mathrm{vol}\bar{X}_j}{\mathrm{vol}X_i\ \mathrm{vol}X_j}}}{\log \frac{\lambda_{n-1}+\lambda_k}{\lambda_{n-1}-\lambda_k}} \right\rceil$$

if $\lambda_k \neq \lambda_{n-1}$ and $X_i \neq \bar{X}_j$.

Another useful generalization of Theorem 3.10 is the following:

THEOREM 3.12. *For $X_i \subset V(G), i = 0, 1, \ldots, k$, we have*

$$\min_{i\neq j} d(X_i, X_j) \leq \min_{0\leq j<k} \max_{i\neq j} \left\lceil \frac{\log \sqrt{\frac{\mathrm{vol}\bar{X}_i\ \mathrm{vol}\bar{X}_j}{\mathrm{vol}X_i\ \mathrm{vol}X_j}}}{\log \frac{\lambda_{n-j-1}+\lambda_{k-j}}{\lambda_{n-j-1}-\lambda_{k-j}}} \right\rceil$$

where j satisfies $\lambda_{k-j} \neq \lambda_{n-j-1}$ and $X_i \neq \bar{X}_j$.

PROOF. For each j, $1 \leq j \leq k-1$, we can use a very similar proof to that of Theorem 3.10 to show that there are two of the subsets with their corresponding vectors satisfying

$$\sum_{i\in S}(1-\lambda_i)^t a_i b_i \geq 0$$

where $S = \{i : 1 \leq i \leq k-j \text{ or } n-j+1 \leq i \leq n-1\}$. The proof then follows. □

3.4. Eigenvalue upper bounds for manifolds

There are many similarities between the Laplace operator on compact Riemannian manifolds and the Laplacian for finite graphs. While the Laplace operator for a manifold is generated by the Riemannian metric, for a graph it comes from the adjacency relation. Sometimes it is possible to treat both the continuous and discrete cases by a universal approach. The general setting is as follows:

(1) An underlying space M with a finite measure μ;
(2) A well-defined Laplace operator $\mathcal{L}$ on functions on M so that $\mathcal{L}$ is a self-adjoint operator in $L^2(M,\mu)$ with a discrete spectrum;

(3) If M has a boundary then the boundary condition should be chosen so that it does not disrupt the self-adjointness of $\mathcal{L}$;
(4) A distance function $\mathrm{dist}(x, y)$ on M so that $|\nabla \mathrm{dist}| \le 1$ for an appropriate notion of gradient.

For a finite connected graph (also denoted by M in this section), the metric μ can be defined to be the degree of each vertex. Together with the Laplacian $\mathcal{L}$, all the above properties are satisfied. In addition, we can consider an r-neighborhood of the support, $\mathrm{supp}_r f$, of a function f in $L^2(M, \mu)$ for $r \in \mathbb{R}$:

$$\mathrm{supp}_r\ f = \{x \in M : \mathrm{dist}(x, \mathrm{supp}\ f) \le r\}$$

where dist denotes the distance function in M. For a polynomial of degree s, denoted by p_s, then we have

$$\mathrm{supp}\ p_s(\mathcal{L})f \subset \mathrm{supp}_s f. \tag{3.6}$$

Let M be a complete Riemannian manifold with finite volume and let $\mathcal{L}$ be the self-adjoint operator $-\Delta$, where Δ is the Laplace operator associated with the Riemannian metric on M (which will be defined later in (3.10), also see [**259**]). Or, we could consider a compact Riemannian manifold M with boundary and let $\mathcal{L}$ be a self-adjoint operator $-\Delta$ subject to the Neumann or Dirichlet boundary conditions (defined in (3.11)). We can still have the following analogous version of (3.6) for the s-neighborhood of the support of a function.

There exists a nontrivial family of bounded continuous functions $P_s(\lambda)$ defined on the spectrum $\mathrm{Spec}\mathcal{L}$*, where s ranges over* $[0, +\infty)$*, so that for any function $f \in L^2(M, \mu)$:*

$$\mathrm{supp} P_s(\mathcal{L})f \subset \mathrm{supp}_s f. \tag{3.7}$$

For example, we can choose $P_s(\lambda) = \cos(\sqrt{\lambda}s)$ which clearly satisfies the requirement in (3.7).

Let us define

$$p(s) = \sup_{\lambda \in \mathrm{Spec}\mathcal{L}} |\ P_s(\lambda)\ |$$

and assume that $p(s)$ is locally integrable.

We consider

$$\Phi(\lambda) = \int_0^\infty \phi(s) P_s(\lambda) ds$$

where $\phi(s)$ is a measurable function on $(0, +\infty)$ such that

$$\int_0^\infty |\phi(s)| p(s) ds < \infty.$$

In particular, $\Phi(\lambda)$ is a bounded function on $\mathrm{Spec}\mathcal{L}$, and we can apply the operator $\Phi(\mathcal{L})$ to any function in $L^2(M, \mu)$.

We will prove the following general lemma which will be useful later.

LEMMA 3.13. *If $f \in L^2(M,\mu)$ then*

$$\|\Phi(\mathcal{L})f\|_{L^2(M\setminus \mathrm{supp}_r f)} \le \|f\|_2 \int_r^\infty |\phi(s)| p(s) ds$$

where $\|f\|_2 := \|f\|_{L^2(M,\mu)}$.

PROOF. Let us denote

$$w(x) = \Phi(\mathcal{L})f(x) = \int_0^\infty \phi(s) P_s(\mathcal{L}) f(x) ds.$$

If the point x is not in $\mathrm{supp}_r f$ then $P_s(\mathcal{L})f(x) = 0$ whenever $s \le r$. Therefore, for those points

$$w(x) = \int_r^\infty \phi(s) P_s(\mathcal{L}) f(x) ds$$

and

$$\begin{aligned} \|w\|_{L^2(M\setminus \mathrm{supp}_r f)} &\le \left\| \int_r^\infty \phi(s) P_s(\mathcal{L}) f(x) ds \right\|_2 \\ &\le \int_r^\infty \|\phi(s) P_s(\mathcal{L}) f(x)\|_2 ds \\ &\le \int_r^\infty |\phi(s)| p(s) \|f\|_2 ds. \end{aligned}$$

The proof is complete. □

As an immediate consequence, we have

COROLLARY 3.14. *If $f, g \in L^2(M,\mu)$ and the distance between* supp f *and* supp g *is D, then*

$$\left| \int_M f \Phi(\mathcal{L}) g d\mu \right| \le \|f\|_2 \|g\|_2 \int_D^\infty |\phi(s)| p(s) ds. \tag{3.8}$$

The integral on the left-hand side of (3.8) is reduced to one over the support of g which in turn is majorized by the integral over the exterior of $\mathrm{supp}_D f$. The rest of the proof follows by a straightforward application of the Cauchy-Schwarz inequality.

For the choice of $P_s(\lambda) = \cos(\sqrt{\lambda} s)$, suppose we select

$$\phi(s) = \frac{1}{\sqrt{\pi t}} e^{-\frac{s^2}{4t}}.$$

Then we have

$$\Phi(\lambda) = \int_0^\infty \phi(s) P_s(\lambda) ds = e^{-\lambda t}.$$

COROLLARY 3.15. *If $f, g \in L^2(M,\mu)$ and the distance between the supports of f and g is equal to D then*

$$\left| \int_M f e^{-t\mathcal{L}} g d\mu \right| \le \|f\|_2 \|g\|_2 \int_D^\infty \frac{1}{\sqrt{\pi t}} e^{-\frac{s^2}{4t}} ds. \tag{3.9}$$

Let us mention a similar but weaker inequality:

COROLLARY 3.16.

$$\left|\int_M fe^{-t\mathcal{L}}gd\mu\right| \le \|f\|_2\|g\|_2e^{-\frac{D^2}{4t}}.$$

This inequality was proved in [**96**] [**259**] and is quite useful.

Let M be a smooth connected compact Riemannian manifold and Δ be a Laplace operator associated with the Riemannian metric, i.e., in coordinates x_1, $x_2, \ldots, x_n$,

$$\Delta u = \frac{1}{\sqrt{g}}\sum_{i,j=1}^{n}\frac{\partial}{\partial x_i}\left(\sqrt{g}g^{ij}\frac{\partial u}{\partial x_j}\right) \tag{3.10}$$

where g^{ij} are the contravariant components of the metric tensor, $g = \det\|g_{ij}\|$, $g^{ij} = \|g_{ij}\|^{-1}$, and u is a smooth function on M.

If the manifold M has a boundary ∂M, we introduce a boundary condition

$$\alpha u + \beta\frac{\partial u}{\partial \nu} = 0 \tag{3.11}$$

where $\alpha(x), \beta(x)$ are non-negative smooth functions on M such that $\alpha(x)+\beta(x) > 0$ for all $x \in \partial M$.

For example, both Dirichlet and Neumann boundary conditions satisfy these assumptions.

The operator $\mathcal{L} = -\Delta$ is self-adjoint and has a discrete spectrum in $L^2(M, \mu)$, where μ denotes the Riemannian measure. Let the eigenvalues be denoted by $0 = \lambda_0 < \lambda_1 \le \lambda_2 \le \cdots$. Let $\mathrm{dist}(x, y)$ be a distance function on $M \times M$ which is Lipschitz and satisfies

$$|\nabla \mathrm{dist}(x, y)| \le 1$$

for all $x, y \in M$. For example, $\mathrm{dist}(x, y)$ may be taken to be the geodesic distance, but we don't necessarily assume this is the case.

We want to show the following (also see [**78**]):

THEOREM 3.17. *For two arbitrary measurable disjoint sets X and Y on M, we have*

$$\lambda_1 \le \frac{1}{\mathrm{dist}(X, Y)^2}\left(1 + \log\frac{(\mu M)^2}{\mu X \mu Y}\right)^2. \tag{3.12}$$

Moreover, if we have $k + 1$ disjoint subsets $X_0, X_1, \ldots, X_k$ such that the distance between any pair of them is greater than or equal to $D > 0$, then we have for any $k \ge 1$,

$$\lambda_k \le \frac{1}{D^2}(1 + \sup_{i\ne j}\log\frac{(\mu M)^2}{\mu X_i\ \mu X_i})^2. \tag{3.13}$$

PROOF. Let us denote by ϕ_i the eigenfunction corresponding to the ith eigenvalue λ_i and normalized in $L^2(M, \mu)$ so that $\{\phi_i\}$ is an orthonormal frame in $L^2(M, \mu)$. For example, if either the manifold has no boundary or the Dirichlet or Neumann boundary condition is satisfied, there is one eigenvalue 0 with the associated eigenfunction being the constant function:

$$\phi_0 = \frac{1}{\sqrt{\mu M}}.$$

The proof is based upon two fundamental facts about the heat kernel $p(x, y, t)$, which by definition is the unique fundamental solution to the heat equation

$$\frac{\partial}{\partial t}u(x,t) - \Delta u(x,t) = 0$$

with the boundary condition (3.11) if the boundary ∂M is non-empty. The first fact is the eigenfunction expansion

$$p(x,y,t) = \sum_{i=0}^{\infty} e^{-\lambda_i t}\phi_i(x)\phi_i(y) \tag{3.14}$$

and the second is the following estimate (by using Corollary 3.16):

$$\int_X \int_Y p(x,y,t)f(x)g(y)\mu(dx)\mu(dy) \leq \left(\int_X f^2 \int_Y g^2\right)^{\frac{1}{2}} e^{-\frac{D^2}{4t}} \tag{3.15}$$

for any functions $f, g \in L^2(M, \mu)$ and for any two disjoint Borel sets $X, Y \subset M$ where $D = \operatorname{dist}(X, Y)$.

We first consider the case $k = 2$. We start by integrating the eigenvalue expansion (3.14) as follows:

(3.16)

$$I(f,g) \quad \equiv \quad \int_X \int_Y p(x,y,t)f(x)g(y)\mu(dx)\mu(dy) = \sum_{i=0}^{\infty} e^{-\lambda_i t}\int_X f\phi_i \int_Y g\phi_i.$$

We denote by f_i the Fourier coefficients of the function $f\psi_X$ with respect to the frame $\{\phi_i\}$ and by g_i those of $g\ \psi_Y$. Then

$$\begin{aligned} I(f,g) &= e^{-\lambda_0 t} f_0 g_0 + \sum_{i=1}^{\infty} e^{-\lambda_i t} f_i g_i \\ &\geq e^{-\lambda_0 t} f_0 g_0 - e^{-\lambda_1 t}\|f\psi_X\|_2 \|g\psi_Y\|_2 \end{aligned}$$

where we have used

$$\left|\sum_{i=1}^{\infty} e^{-\lambda_i t} f_i g_i\right| \leq e^{-\lambda_1 t}\left(\sum_{i=1}^{\infty} f_i^2 \sum_{i=1}^{\infty} g_i^2\right)^{\frac{1}{2}} \leq e^{-\lambda_1 t}\|f\psi_X\|_2\|g\psi_Y\|_2.$$

By comparing (3.17) and (3.15), we have

(3.17)

$$e^{-\lambda_1 t}\|f\psi_X\|_2\ \|g\psi_Y\|_2 \quad \geq \quad f_0 g_0 - \|f\psi_X\|_2\ \|g\psi_Y\|_2 e^{-\frac{D^2}{4t}}.$$

We will choose t so that the second term on the right-hand side of (3.17) is equal to one half of the first one (here we take advantage of the Gaussian exponential since it can be made arbitrarily close to 0 by taking t small enough):

$$t = \frac{D^2}{4 \log \frac{2\|f\psi_X\|_2\ \|g\psi_Y\|_2}{f_0 g_0}}.$$

For this t we have

$$e^{-\lambda_1 t}\|f\psi_X\|_2\|g\psi_Y\|_2 \geq \frac{1}{2}f_0g_0$$

which implies

$$\lambda_1 \leq \frac{1}{t}\log\frac{2\|f\psi_X\|_2\ \|g\psi_Y\|_2}{f_0g_0}.$$

After substituting this value of t, we have

$$\lambda_1 \leq \frac{4}{D^2}\left(\log\frac{2\|f\psi_X\|_2\ \|g\psi_Y\|_2}{f_0g_0}\right)^2.$$

Finally, we choose $f = g = \phi_0$ and take into account that

$$f_0 = \int_X f\phi_0 = \int_X \phi_0^2,$$

and

$$\|f\psi_X\|_2 = \left(\int_X \phi_0^2\right)^{\frac{1}{2}} = \sqrt{f_0}.$$

Similar identities hold for g. We then obtain

$$\lambda_1 \leq \frac{1}{D^2}\left(\log\frac{4}{\int_X \phi_0^2 \int_Y \phi_0^2}\right)^2.$$

Now we consider the general case $k > 2$. For a function $f(x)$, we denote by f_i^j the i-th Fourier coefficient of the function $f\mathbf{1}_{X_j}$ i.e.

$$f_i^j = \int_{X_j} f\phi_i.$$

Similar to the case of $k = 2$, we have

$$I_{lm}(f,f) = \int_{X_l}\int_{X_m} p(x,y,t)f(x)f(y)\mu(dx)\mu(dy).$$

Again, we have the following upper bound for $I_{lm}(f,f)$:

$$I_{lm}(f,f) \leq \|f\psi_{X_l}\|_2\ \|f\psi_{X_m}\|_2 e^{-\frac{D^2}{4t}}. \tag{3.18}$$

We can rewrite the lower bound (3.17) in another way:

(3.19)

$$I_{lm}(f,f) \quad \geq \quad e^{-\lambda_0 t}f_0^l f_0^m + \sum_{i=1}^{k-1} e^{-\lambda_i t} f_i^l f_i^m - e^{-\lambda_k t}\|f\psi_{X_l}\|_2\ \|f\psi_{X_m}\|_2.$$

Now we can eliminate the middle term on the right-hand side of (3.19) by choosing appropriate l and m. To this end, let us consider $k+1$ vectors $f^m = (f_1^m, f_2^m, \ldots, f_{k-1}^m)$, $m = 0, 1, 2, \ldots, k$ in $\mathbb{R}^{k-1}$ and let us endow this $(k-1)$-dimensional space with a scalar product given by

$$(v, w) = \sum_{i=1}^{k-1} v_i w_i e^{-\lambda_i t}.$$

By using Corollary 3.9, out of any $k+1$ vectors in $(k-1)$-dimensional Euclidean space there are always two vectors with non-negative scalar product. So, we can find different l, m so that $\langle f^l, f^m\rangle \geq 0$ and therefore we can eliminate the second term on the right-hand side (3.19).

Comparing (3.18) and (3.19), we have

(3.20)

$$e^{-\lambda_k t}\|f\psi_{X_l}\|_2 \ \|f\psi_{X_m}\|_2 \quad \leq \quad f_0^l f_0^m - \|f\psi_{X_l}\|_2 \ \|f\psi_{X_m}\|_2 e^{-\frac{D^2}{4t}}.$$

Similar to the case $k = 2$, we can choose t so that the right-hand side is at least $\frac{1}{2}f_0^l f_0^m$. We select

$$t = \min_{l \neq m} \frac{D^2}{4 \log \frac{2\|f\psi_{X_l}\|_2 \|f\psi_{X_m}\|_2}{f_0^l f_0^m}}.$$

From (3.20), we have

$$\lambda_k \leq \frac{1}{t} \log \frac{2\|f\psi_{X_l}\|_2 \ \|f\psi_{X_m}\|_2}{f_0^l f_0^m}.$$

By substituting t from above and taking $f = \phi_0$, (3.13) follows. □

Although differential geometry and spectral graph theory share a great deal in common, there is no question that significant differences exist. Obviously, a graph is not "differentiable" and many geometrical techniques involving high-order derivatives could be very difficult, if not impossible, to utilize for graphs. There are substantial obstacles for deriving the discrete analogues of many of the known results in the continuous case. Nevertheless, there are many successful examples of developing the discrete parallels, and this process sometimes leads to improvement and strengthening of the original results from the continuous case. Furthermore, the discrete version often offers a different viewpoint which can provide additional insight to the fundamental nature of geometry. In particular, it is useful in focusing on essentials which are related to the global structure instead of the local conditions.

There are basically two approaches in the interplay of spectral graph theory and spectral geometry. One approach, as we have seen in this section, is to share the concepts and methods while the proofs for the continuous and discrete, respectively, remain self-contained and independent. The second approach is to approximate the discrete cases by continuous ones. This method is usually coupled with appropriate assumptions and estimates. One example of this approach will be given in Chapter 10.

For almost every known result in spectral geometry, a corresponding set of questions can be asked: Can the results be translated to graph theory? Is the discrete analogue true for graphs? Do the proof techniques still work for the discrete case? If not, how should the methods be modified? If the discrete analogue does not hold for general graphs, can it hold for some special classes of graphs? What are the characterizations of these graphs?

Discrete invariants are somewhat different from the continuous ones. For example, the number of vertices n is an important notion for a graph. Although it can be roughly identified as a quantity which goes to infinity in the continuous analog, it is of interest to distinguish $n, n \log n, n^2, \ldots$ and 2^n, for example. Therefore more careful analysis is often required. For Riemannian manifolds, the dimension of the manifold is usually given and can be regarded as a constant. This is however not true in general for graphs. The interaction between spectral graph theory and differential geometry opens up a whole range of interesting problems.

Notes

This chapter is based on the original diameter-eigenvalue bounds given in [**59**] and a subsequent paper [**65**]. The generalizations to pairs of subsets for regular graphs were given by Kahale in [**171**]. The generalizations to k subsets and to Riemannian manifolds can be found in [**78, 79**].