Eigenvalues of graphs*

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1   Introduction

The study of eigenvalues of graphs has a long history. From the early days, representation theory and number theory have been very useful for examining the spectra of strongly regular graphs with symmetries. In contrast, recent developments in spectral graph theory concern the effectiveness of eigenvalues in studying general (unstructured) graphs. The concepts and techniques, in large part, use essentially geometric methods. (Still, extremal and explicit constructions are mostly algebraic[19]). There has been a significant increase in the interaction between spectral graph theory and many areas of mathematics as well as other disciplines, such as physics, chemistry, communication theory and computer science.

In this paper, we will briefly describe some recent advances in the following three directions.

1. The connections of eigenvalues to graph invariants such as diameter, distances, flows, routing, expansion, isopermetric properties, discrepancy, containment and, in particular, the role eigenvalues play in the equivalence classes of so-called "quasi-random" properties.

2. The techniques of bounding eigenvalues and eigenfunctions, with special emphasis on the Sobolev and Harnack inequalities for graphs.

3. Eigenvalue bounds for special families of graphs, such as the convex subgraphs of homogeneous graphs, with applications to random walks and efficient approximation algorithms.

This paper is organized as follows. Section 2 includes some basic definitions. In Section 3, we discuss the relationship of eigenvalues to graph invariants. In Section 4 we describe the consequences and limitations of the Sobolev and Harnack inequalities. In Section 5, we use the heat kernel to derive eigenvalue lower bounds which are especially useful for the case of convex subgraphs. In Section 6 some examples and applications are illustrated. Since all proofs will not be included here and the statements can sometimes be very brief, the reader is referred to [12] for more discussion and details.

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2 Preliminaries

In a graph G with vertex set $V = V(G)$ and edge set $E = E(G)$, we define the Laplacian $\mathcal{L}$ as a matrix with rows and columns indexed by V as follows:

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

where d_v denotes the degree of v. Here we consider simple, loopless graphs (since all results can be easily extended to general weighted graphs with loops [12].) For k-regular graphs, it is easy to see that

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

where A is the adjacency matrix. For a general graph, we have

$$\mathcal{L} = I - T^{-\frac{1}{2}} A T^{-\frac{1}{2}}$$

where T is the diagonal matrix with value d_v at the (v,v)-entry. The eigenvalues of $\mathcal{L}$ are denoted by

$$0 = \lambda_0 \le \lambda_1 \le \cdots \le \lambda_{n-1}$$

and

$$\lambda_G := \lambda_1 = \inf_{\substack{f \\ \sum f(v)d_v = 0}} \frac{\displaystyle\sum_{u \sim v}(f(u) - f(v))^2}{\displaystyle\sum_v f(v)^2 d_v}$$

$$= \inf_{\substack{h \\ \sum h(v)\sqrt{d_v} = 0}} \frac{\langle h, \mathcal{L}h \rangle}{\langle h, h \rangle}$$

In a way, the eigenvalues λ_i's can be viewed as the discrete analogues of the Laplace-Beltrami operator for Riemannian manifolds

$$\lambda_M = \inf_f \frac{\displaystyle\int_M ||\nabla f||^2}{\displaystyle\int_M ||f||^2}$$

where f ranges over functions satisfying $\int_M f = 0$. For a connected graph G, we have $\lambda_G > 0$ and in general $0 \le \lambda_G \le 1$, with the exception of $G = K_n$, the complete graph (in which case $\lambda_G = n/(n-1)$). Also $1 < \lambda_{n-1} \le 2$, with equality holding for bipartite graphs.

3 Eigenvalues and graph properties

In a graph G on n vertices, the distance between two vertices u and v, denoted by $d(u,v)$ is the length of a shortest path joining u and v. The diameter of G, denoted by $D(G)$, is the maximum distance over all pairs of vertices: A lower bound for λ_1 implies an upper bound for $D(G)$. Namely, in [6], it was shown that for regular graphs, we have

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

with the exception of the complete graph K_n. (We assme in this section that $G \neq K_n$ and G is connected.) The proof is based on the simple observation that $D(G) \leq t$ if, for some polynomial P_t of degree t and some $n \times n$ matrix M with $M(u,v) = 0$ for $u \not\sim v$, we have all entries of $P_t(M)$ nonzero. The above inequality can be further extended for distances between any two subsets X, Y of vertices in G. Here we denote the distance $d(X,Y)$ to be the minimum distance between a vertex in X and a vertex in Y.

$$d(X,Y) \leq \left\lceil \frac{\log \frac{vol\ V}{vol\ X vol\ Y}}{\log \frac{1}{1-\lambda'}} \right\rceil \tag{2}$$

where the volume of a subset X is defined to be $vol\ X = \sum_{v \in X} d_v$, and λ' is equal to λ_1 if $1 - \lambda_1 \geq \lambda_{n-1} - 1$, or else $\lambda' = 2\lambda_1/(\lambda_1 + \lambda_{n-1})$. The above inequalities have several generalizations. For example, the distances among $k+1$ subsets $X_1, \cdots, X_{k+1}$ of V are related to the k-th eigenvalue λ_k for $k \geq 2$.

$$\min_{i \neq j} d(X_i, X_j) \leq \max_{i \neq j} \left\lceil \frac{\log \frac{vol\ V}{vol\ X_i vol\ X_j}}{\log \frac{1}{1-\lambda_k}} \right\rceil \tag{3}$$

if $1 - \lambda_k \geq \lambda_{n-1} - 1$; otherwise replace λ_k by $\frac{2\lambda_k}{\lambda_k + \lambda_{n-1}}$ in (3).

This can be further generalized to eigenvalue bounds for a Laplace operator on a smooth, connected, compact Riemannian manifold M [15]:

$$\lambda_k \leq \frac{4}{t^2} \max_{i \neq j} \left(\log \frac{2\ vol\ M}{\sqrt{vol\ X_i vol\ X_j}} \right)^2 \tag{4}$$

if there are $k+1$ disjoint subsets $X_1, \cdots, X_{k+1}$ such that the geodesic distance between any pair of them is at least t.

The above inequalities can be used to derive isoperimetric inequalities in the following way. For a subset X of vertices, we define the t-boundary $\delta_t(X) = \{u \notin X : d(u,v) \leq t$ for some $v \in X\}$. By substituting $Y = V - \delta_t(X) - X$ in (2) we deduce

$$\frac{vol(\delta_t(X))}{vol\ (X)} \geq (1 - (1-\lambda')^{2t})(1 - \frac{vol\ X}{vol\ V}) \tag{5}$$

We remark that the special case of (5) for regular graphs was proved by Alon [1] and Tanner [23].

Another type of boundary for a subset X is

$$\partial(X) = \{\{x, x'\} \in E : x \in X, x' \notin X\}$$

The Cheeger constant h_G is defined to be

$$h_G = \min_{\substack{x \\ |vol\ X| \le \frac{1}{2} vol\ V}} \frac{|\partial(X)|}{vol\ X}$$

and the Cheeger's inequality states

$$2h_G \ge \lambda_1 \ge \frac{h_G^2}{2}.$$

The discrete version of Cheeger's inequality was considered in [17, 3] with proof techniques quite similar to those used for the continuous case by Cheeger [5], and can be traced back to the early work of Polya and Szego [21].

The implications of the above isoperimetric inequalities can be summarized as follows: When λ_1 is bounded away from 0, i.e., $\lambda_1 \ge c > 0$ for some absolute constant c, the diameter is "small" and the boundary of a subset X is "large" (proportional to the volume of the subset). As an immediate consequence of the isoperimetric inequalities, there are many paths with "small" overlap simultaneously joining all pairs of vertices. In fact, the following dynamic version of routing can be achieved efficiently (in logarithmic time in n). Namely, in a regular graph G, suppose pebbles p_i are placed on vertices v_i with destination $v_{\pi(i)}$ for some permutation $\pi \in S_n$. At each step, every pebble is allowed to move along some edge to a neighboring vertex provided that no two pebbles can be placed at the same vertex simultaneously. Then there is a routing scheme to move all pebbles to their destinations in $O(\frac{1}{\lambda^2} \log^2 n)$ time (see [2] and [12]).

When both λ_1 and λ_{n-1} are close to 1, the graph G satisfies additional properties. For example, for two subsets of vertices, say X and Y, the number $e(X, Y)$ of pairs (x, y), $x \in X$, $y \in Y$ and $\{x, y\} \in E$, is close to the expected value. Here by "expected" value, we mean the expected value for a random graph with the same edge density. To be precise, we have the following inequality:

$$|e(X, Y) - \frac{vol\ X vol\ Y}{vol\ V}| \le \max_{i \ne 0} |1 - \lambda_i| \sqrt{vol\ X vol\ Y}$$

When $X = Y$, the left hand side of the above inequality is called the discrepancy of X.

For sparse graphs, say k-regular graphs for some fixed k, $1 - \lambda_1$ cannot be too small. In fact, $1 - \lambda_1 \ge \frac{1}{\sqrt{k}}$. However for dense graphs, $1 - \lambda_1$ can be very close to zero. For example, almost all graphs have $1 - \lambda_1$ at most $\frac{c}{\sqrt{n}}$. For graphs with constant edge density, say $\rho = \frac{1}{2}$, the condition of $1 - \lambda_1 = o(1)$ implies many strong graph properties. Here we will use descriptions of graph properties containing the $o(1)$ notation so that $P(o(1)) \to P'(o(1))$ means that for any $\epsilon > 0$,

there exists δ such that $P(\delta) \to P'(\epsilon)$. Two properties P and P' are equivalent if $P \to P'$ and $P' \to P$. The following class of properties for an almost regular graph G, with edge density $\frac{1}{2}$, have all been shown to be equivalent [14] (also see [12]) and this class of graph properties is termed "quasi-random" since a random graph shares these properties.

P_1: $\max_{i>0} |1 - \lambda_i| = o(1)$

P_2: For any subset X of vertices, discrepancy of $X = o(1) \cdot vol\, X$.

For a fixed $s \geq 4$,

$P_3(s)$: For any graph H on s vertices, the number of occurrences of H as an induced subgraph of G is $(1 + o(1))$ times the expected number.

P_4 : For almost all pairs x, y of vertices, the number of vertices w satisfies ($w \sim x$ and $w \sim y$) or ($w \not\sim x$ and $w \not\sim y$) is $(1 + o(1))$ times the expected number.

We remark that the $o(1)$ terms in the above properties represent the estimates of deviations from the expectation. The problems of determining the order and the behavior of these deviations and the relations between various estimates touch many aspects of extremal graph theory and random graph theory. Needless to say, many intriguing questions remain open. We remark that quasi-random classes for hypergraphs have also been established and examined in [13].

4 Sobolev and Harnack inequalities

In this section, we will describe the Sobolev inequalities and Harnack inequalities for eigenfunctions of graphs which then lead to eigenvalue bounds. The ideas and proof techniques are quite similar to various classical methods in treating the eigenvalues of connected smooth compact Riemannian manifolds. In general, there are often various obstructions to applying continuous methods in the discrete domain. For example, many differential techniques can be quite hard to utilize since the eigenfunctions for graphs are defined on a finite number of vertices and the task of taking derivatives can therefore be difficult (if not impossible). Furthermore, general graphs usually represent all possible configurations of edges, and, as a consequence, many theorems concerning smooth surfaces are simply not true for graphs. Nevertheless, there are many common concepts that provide connections and interactions between spectral graph theory and Riemannian geometry. As a successful example, the Sobolev inequalities for graphs can be proved almost entirely by classical techniques which can be traced back to Nash [25]. The situation for the Harnack inequalities for graphs is somewhat different since discrete versions of the statement for the continuous cases do not hold in general. However, we will describe a Harnack inequality which works for eigenfunctions of homogeneous graphs and some special subgraphs that we call "strongly convex."

We first consider Sobolev inequalities which holds for all general graphs. To start with, we define a graph invariant, the so-called isopermetric dimension, which is involved in the Sobolev inequality.

We say that a graph G has isoperimetric dimension δ with an isoperimetric constant c_δ if for all subsets X of $V(G)$, the number of edges between X and the complement $\bar{X}$ of X, denoted by $e(X, \bar{X})$, satisfies

$$e(X, \bar{X}) \geq c_\delta (vol\ X)^{\frac{\delta-1}{\delta}}$$

where $vol\ X \leq vol\ \bar{X}$ and c_δ is a constant depending only on δ. Let f denote an arbitray function $f : V(G) \to \mathbf{R}$. The following Sobolev inequalities hold.

(i) For $\delta > 1$,

$$\sum_{u \sim v} |f(u) - f(v)| \geq c_\delta \frac{\delta-1}{\delta} \min_m (\sum_v |f(v) - m|^{\frac{\delta}{\delta-1}} d_v)^{\frac{\delta-1}{\delta}}$$

(ii) For $\delta > 2$,

$$(\sum_{u \sim v} |f(u) - f(v)|^2)^{\frac{1}{2}} \geq c_\delta \frac{\delta-1}{\sqrt{2\delta}} \min_m (\sum_v |(f(v) - m)^\alpha d_v)^{\frac{1}{\alpha}}$$

where $\alpha = \frac{2\delta}{\delta-2}$.

The above two inequalities can be used to derive the following eigenvalue inequalities for a graph G (see [9]):

$$\sum_{i>0} e^{-\lambda_i t} \leq c \frac{vol\ V}{t^{\frac{\delta}{2}}} \tag{6}$$

$$\lambda_k \geq c' (\frac{k}{vol\ V})^{\frac{2}{\delta}} \tag{7}$$

for suitable contants c and c' which depend only on δ.

In a way, a graph can be viewed as a discretization of a Riemannian manifold in $\mathbf{R}^n$ where n is roughly equal to δ. The eigenvalue bounds in (7) are analogues of the Polya conjecture for Dirichlet eigenvalues of a regular domain M.

$$\lambda_k \geq \frac{2\pi}{w_n} (\frac{k}{vol\ M})^{\frac{2}{n}}$$

where w_n is the volume of the unit disc in $\mathbf{R}^n$.

From now on, we assume that f is an eigenfunction of the Laplacian of G. The usual Harnack inequality concerns establishing an upper bound for the quantity $\max_{x \sim y}(f(x) - f(y))^2$ by a multiple of λ and $\max_x f^2(x)$. Such an inequality does not hold for general graphs, (for example, for the graph formed by joining two complete graphs K_n by an edge.) We will show that we can have a Harnack inequality for certain homogeneous graphs and some of their subgraphs.

A homogeneous graph is a graph Γ together with a group H acting on the vertices satisfying:

1. For any $g \in H, u \sim v$ if and only if $gu \sim gv$.

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2. For any $u, v \in V(\Gamma)$ there exists $g \in H$ such that $gu = v$.

In other words, Γ is vertex transitive under the action of H and the vertices of Γ can be labelled by cosets H/I where $I = \{g | gv = v\}$ for a fixed v. Also, there is an edge generating set $K \subset H$ such that for all vertices $v \in V(\Gamma)$ and $g \in K$, we have $\{v, gv\} \in E(\Gamma)$.

A homogeneous graph is said to be invariant if K is invariant as a set under conjugation by elements of K, i.e., for all $a \in K$, $aKa^{-1} = K$.

Let f denote an eigenfunction in an invariant homogeneous graph with edge generating set K consisting of k generators. Then it can be shown [10] that

$$\frac{1}{k} \sum_{a \in K} (f(x) - f(ax))^2 \leq 8\lambda \sup_y f^2(y)$$

An induced subgraph S of a graph Γ is said to be *strongly convex* if for all pairs of vertices u and v in S, all shortest paths joining u and v in Γ are contained in S. The main theorem in [10] asserts that the following Harnack inequality holds.

Suppose S is a strongly convex subgraph in an abelian homogeneous graph with edge generating set K consisting of k generators. Let f denote an eigenfunction of S associated with the Neumann eigenvalue λ. Then for all $x \in S$, $x \sim y$,

$$|f(x) - f(y)|^2 \leq 8k\lambda \sup_{z \in S} f^2(z)$$

The Neumann eigenvalues for subgraphs will be defined in the next section. A direct consequence of the Harnack inequalities is the following lower bound for the Neumann eigenvalue λ of S:

$$\lambda \geq \frac{1}{8kD^2}$$

where k is the maximum degree and D is the diameter of S. Such eigenvalue bounds are particularly useful for deriving polynomial approximation algorithms when enumeration problems of combinatorial structures can often be represented as random walk problems on "convex" subgraphs of appropriate homogeneous graphs. However, the condition of strongly convex subgraph poses quite severe constraints, which will be relaxed in the next section.

5 Eigenvalue inequalities for subgraphs and convex subgraphs

Let S denote a subset of vertices in G. An induced subgraph on S consists of all edges with both end points in S. While a graph corresponds to a manifold with no boundary, an induced subgraph on S can then be associated with a submanifold with a boundary. Next, we define the Neumann eigenvalue for an induced subgraph on S. Let $\hat{S}$ denote the extension of S formed by all edges with at least one end

point in S. The Neumann eigenvalue λ_S for S is defined to be

$$\lambda_S = \inf_f \frac{\displaystyle\sum_{\{x,y\}\in\hat{S}} (f(x) - f(y))^2}{\displaystyle\sum_{x\in S} f^2(x)d_x} = \inf_g \frac{\langle g, \mathcal{L}g\rangle}{\langle g, g\rangle}$$

where f ranges over all functions $f : S \cup \delta S \to \mathbf{R}$ satisfying $\displaystyle\sum_{x\in S} f(x)d_x = 0$, $g(x) = f(x)\sqrt{d_x}$ and $\mathcal{L}$ denotes the Laplacian of S.

Let ϕ_i denote the eigenfunction for the Laplacian corresponding to eigenvalue λ_i. Then ϕ_i satisfies

$$\mathcal{L}\phi_i(x) = \begin{cases} \lambda_i\phi_i(x) & \text{if } x \in S \\ 0 & \text{if } x \in \delta S \end{cases}$$

We now define the heat kernel of S as a $n \times n$ matrix

$$
\begin{aligned}
H_t &= \sum e^{\lambda_i t} P_i \\
&= e^{-t\mathcal{L}} \\
&= I - t\mathcal{L} + \frac{\sum^2}{2}\mathcal{L} + \cdots
\end{aligned}
$$

where $\mathcal{L} = \sum \lambda_i P_i$ is the decomposition of the Laplacian $\mathcal{L}$ into projections on its eigenspaces. In particular, we have

- $H_0 = I$

- $F(x,t) = \displaystyle\sum_{y\in S\cup\delta S} H_t(x,y)f(y) = (H_t f)(x)$

- $F(x,0) = f(x)$

- F satisfied the heat equation

$$\frac{\partial F}{\partial t} = -\mathcal{L}F$$

- $H_t(x,y) \geq 0$

By using the heat kernel, the following eigenvalue inequality can be derived, for all $t > 0$:

$$\lambda_S \geq \frac{\displaystyle\sum_{x\in S} \inf_{y\in S} H_t(x,y)\frac{\sqrt{d_x}}{\sqrt{d_y}}}{2t}.$$

One way to use the above theorem is to bound the heat kernel of a graph by the (continuous) heat kernel of the Riemannian manifolds, for certain graphs that we call convex subgraphs. We say Γ is a lattice graph if Γ is embedded into a d-dimensional Riemannian manifold $\mathcal{M}$ with a metric μ such that $\epsilon = \mu(x, gx) = \mu(y, g'y)$ for all $g, g' \in K$. An induced subgraph of a homogeneous graph Γ is said to be convex if the following conditions are satisfied:

1. There is a submanifold $M \subset \mathcal{M}$ with a convex boundary such that

$$V(\Gamma) \cap M - \partial M = S$$

2. For any $x \in S$, the ball centered at x of S of radius $\epsilon/2$ is contained in M.

We need one more condition to apply our theorem on convex subgraphs. Basically, ϵ has to be "small" enough so that the count of vertices in S can be used to approximate the volume of the manifold M. Namely, let us define

$$r = \frac{U \; |S|}{vol \; M} \tag{8}$$

where U denotes the volume of *Vononoi* region which consists of all points in $\mathcal{M}$ closest to a lattice point. Then the main result in [11] states that the Neumann eigenvalue of S satisfies the following inequality:

$$\lambda_1 \geq \frac{c \; r \; \epsilon^2}{d^2 D^2(M)}$$

for some absolute constant c, which depends only on Γ, and $D(M)$ denotes the diameter of the manifold M. We note that r in (8) can be lower bounded by a constant if the diameter of M measured in L_1 norm is at least as large as ϵd.

6 Applications to random walks and rapidly mixing Markov chains

As an application of the eigenvalue inequalities in the previous sections, we consider the classical problem of sampling and enumerating the family S of $n \times n$ matrices with nonnegative integral entries with given row and column sums. Although the problem is presumed to be computationally intractable, (in the so-called #P-complete class), the eigenvalue bounds in the previous section can be used to obtain a polynomial approximation algorithm. To see this, we consider the homogeneous graph Γ with the vertex set consisting of all $n \times n$ matrices with integral entries (possibly negative) with given row and column sums. Two vertices u and v are adjacent if u and v differ at just the four entries of a 2×2 submatrix with entries $u_{ik} = v_{ik} + 1, u_{jk} = v_{jk} - 1, u_{im} = v_{im} - 1, u_{jm} = v_{jm} + 1$. The family S of matrices with all nonnegative entries is then a convex subgraph of Γ.

On the vertices of S, we consider the following random walk. The probability $\pi(u, v)$ of moving from a vertex u in S to a neighboring vertex v is $\frac{1}{k}$ if v is in S where k is the degree of Γ. If a neighbor v of u (in Γ) is not in S, then we move from u to each neighbor z of v, z in S, with the (additional) probability $\frac{1}{d_v'}$ where $d_v' = |\{z \in S : z \sim v \text{ in } \Gamma\}|$ for $v \notin S$. In other words, for $u, v \in S$,

$$\pi(u, v) = \frac{w_{uv}}{d_u} + \sum_{\substack{z \notin S \\ u \sim z, v \sim z}} \frac{w_{uz}}{d_v d_z'} w_{zv}$$

where w_{uv} denotes the weight of the edge $\{u, v\}$ ($w_{uv} = 1$ or 0 for simple graphs) and $d_u = \sum_{u \sim v} d_{uv}$.

The stationary distribution for this walk is uniform. Let λ_π denote the second largest eigenvalue of π. It can be shown [11] that

$$1 - \lambda_\pi \geq \lambda_S$$

In particular, if the total row sum (minus the maximum row sum) is $\geq c'\ n^2$, we have $1 - \lambda_\pi \geq \frac{c}{kD^2}$. This implies that a random walk converges to the uniform distribution in $O(\frac{1}{1-\lambda_\pi}) = O(k^2 D^2)$ steps (measured in L_2 norm) and in $O(k^2 D^2 (\log n))$ steps for relative pointwise convergence.

It is reasonable to expect that the above techniques can be useful for developing approximation algorithms for many other difficult enumeration problems by considering random walk problems in appropriate convex subgraphs. Further applications using the eigenvalue bounds in previous sections can be found in [15].

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