Eigenvalues of graphs

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1 Background from linear algebra

1.1 Basic facts about eigenvalues

Let A be an $n \times n$ real matrix. An *eigenvector* of A is a vector such that Ax is parallel to x; in other words, $Ax = \lambda x$ for some real or complex number λ. This number λ is called the *eigenvalue* of A belonging to eigenvector v. Clearly λ is an eigenvalue iff the matrix $A - \lambda I$ is singular, equivalently, iff $det(A - \lambda I) = 0$. This is an algebraic equation of degree n for λ, and hence has n roots (with multiplicity).

The *trace* of the square matrix $A = (A_{ij})$ is defined as

$$\mathrm{tr}(A) = \sum_{i=1}^{n} A_{ii}.$$

The trace of A is the sum of the eigenvalues of A, each taken with the same multiplicity as it occurs among the roots of the equation $det(A - \lambda I) = 0$.

If the matrix A is symmetric, then its eigenvalues and eigenvectors are particularly well behaved. All the eigenvalues are real. Furthermore, there is an orthogonal basis $v_1, \ldots, v_n$ of the space consisting of eigenvectors of A, so that the corresponding eigenvalues $\lambda_1, \ldots, \lambda_n$ are precisely the roots of $det(A - \lambda I) = 0$. We may assume that $|v_1| = \cdots = |v_n| = 1$; then A can be written as

$$A = \sum_{i+1}^{n} \lambda_i v_i v_i^{\mathsf{T}}.$$

Another way of saying this is that every symmetric matrix can be written as $U^{\mathsf{T}} D U$, where U is an orthogonal matrix and D is a diagonal matrix. The eigenvalues of A are just the diagonal entries of D.

To state a further important property of eigenvalues of symmetric matrices, we need the following definition. A *symmetric minor* of A is a submatrix B obtained by deleting some rows and the *corresponding* columns.

Theorem 1.1 (Interlacing eigenvalues) *Let A be an $n \times n$ symmetric matrix with eigenvalues $\lambda_1 \geq \cdots \geq \lambda_n$. Let B be an $(n-k) \times (n-k)$ symmetric minor of A with eigenvalues $\mu_1 \geq \cdots \geq \mu_{n-k}$. Then*

$$\lambda_i \leq \mu_i \leq \lambda_{i+k}.$$

We conclude this little overview with a further basic fact about nonnegative matrices.

Theorem 1.2 (Perron-Frobenius) *If an $n \times n$ matrix has nonnegative entries then it has a nonnegative real eigenvalue λ which has maximum absolute value among all eigenvalues. This eigenvalue λ has a nonnegative real eigenvector. If, in addition, the matrix has no block-triangular decomposition (i.e., it does not contain a $k \times (n-k)$ block of 0-s disjoint from the diagonal), then λ has multiplicity 1 and the corresponding eigenvector is positive.*

1.2 Semidefinite matrices

A symmetric $n \times n$ matrix A is called *positive semidefinite*, if all of its eigenvalues are nonnegative. This property is denoted by $A \succeq 0$. The matrix is *positive definite*, if all of its eigenvalues are positive.

There are many equivalent ways of defining positive semidefinite matrices, some of which are summarized in the Proposition below.

Proposition 1.3 *For a real symmetric $n \times n$ matrix A, the following are equivalent:*

(i) *A is positive semidefinite;*

(ii) *the quadratic form $x^T Ax$ is nonnegative for every $x \in \mathbb{R}^n$;*

(iii) *A can be written as the Gram matrix of n vectors $u_1, ..., u_n \in \mathbb{R}^m$ for some m; this means that $a_{ij} = u_i^{\mathsf{T}} u_j$. Equivalently, $A = U^{\mathsf{T}} U$ for some matrix U;*

(iv) *A is a nonnegative linear combination of matrices of the type xx^{T};*

(v) *The determinant of every symmetric minor of A is nonnegative.*

Let me add some comments. The least m for which a representation as in (iii) is possible is equal to the rank of A. It follows e.g. from (ii) that the diagonal entries of any positive semidefinite matrix are nonnegative, and it is not hard to work out the case of equality: all entries in a row or column with a 0 diagonal entry are 0 as well. In particular, the trace of a positive semidefinite matrix A is nonnegative, and $\mathrm{tr}(A) = 0$ if and only if $A = 0$.

The sum of two positive semidefinite matrices is again positive semidefinite (this follows e.g. from (ii) again). The simplest positive semidefinite matrices are of the form aa^T for some vector a (by (ii): we have $x^\mathsf{T}(aa^\mathsf{T})x = (a^\mathsf{T}x)^2 \geq 0$ for every vector x). These matrices are precisely the positive semidefinite matrices of rank 1. Property (iv) above shows that every positive semidefinite matrix can be written as the sum of rank-1 positive semidefinite matrices.

The product of two positive semidefinite matrices A and B is not even symmetric in general (and so it is not positive semidefinite); but the following can still be claimed about the product:

Proposition 1.4 *If A and B are positive semidefinite matrices, then $\mathrm{tr}(AB) \geq 0$, and equality holds iff $AB = 0$.*

Property (v) provides a way to check whether a given matrix is positive semidefinite. This works well for small matrices, but it becomes inefficient very soon, since there are many symmetric minors to check. An efficient method to test if a symmetric matrix A is positive semidefinite is the following algorithm. Carry out Gaussian elimination on A, pivoting always on diagonal entries. If you ever find a negative diagonal entry, or a 0 diagonal entry whose row contains a non-zero, stop: the matrix is not positive semidefinite. If you obtain an all-zero matrix (or eliminate the whole matrix), stop: the matrix is positive semidefinite.

If this simple algorithm finds that A is not positive semidefinite, it also provides a certificate in the form of a vector v with $v^\mathsf{T}Av < 0$. Assume that the i-th diagonal entry of the matrix $A^{(k)}$ after k steps is negative. Write $A^{(k)} = E_k^\mathsf{T} \dots E_1^\mathsf{T} A E_1 \dots E_k$, where E_i are elementary matrices. Then we can take the vector $v = E_1 \dots E_k e_i$. The case when there is a 0 diagonal entry whose row contains a non-zero is similar.

It will be important to think of $n \times n$ matrices as vectors with n^2 coordinates. In this space, the usual inner product is written as $A \cdot B$. This should not be confused with the matrix product AB. However, we can express the inner product of two $n \times n$ matrices A and B as follows:

$$A \cdot B = \sum_{i=1}^{n} \sum_{j=1}^{n} A_{ij} B_{ij} = \mathrm{tr}(A^\mathsf{T} B).$$

Positive semidefinite matrices have some important properties in terms of the geometry of this space. To state these, we need two definitions. A *convex cone* in $\mathbb{R}^n$ is a set of vectors which along with any vector, also contains any positive scalar multiple of it, and along with any two vectors, also contains their sum. Any system of homogeneous linear inequalities

$$a_1^\mathsf{T} x \geq 0, \quad \dots \quad a_m^\mathsf{T} x \geq 0$$

defines a convex cone; convex cones defined by such (finite) systems are called *polyhedral*.

For every convex cone C, we can form its *polar cone* C^*, defined by

$$C^* = \{x \in \mathbb{R}^n : x^\mathsf{T} y \geq 0 \ \forall y \in C\}.$$

This is again a convex cone. If C is closed (in the topological sense), then we have $(C^*)^* = C$.

The fact that the sum of two such matrices is again positive semidefinite (together with the trivial fact that every positive scalar multiple of a positive semidefinite matrix is positive

semidefinite), translates into the geometric statement that *the set of all positive semidefinite matrices forms a convex closed cone* $\mathcal{P}_n$ *in* $\mathbb{R}^{n\times n}$ *with vertex* 0. This cone $\mathcal{P}_n$ is important, but its structure is quite non-trivial. In particular, it is non-polyhedral for $n \geq 2$; for $n = 2$ it is a nice rotational cone (Figure 1; the fourth coordinate x_{21}, which is always equal to x_{12} by symmetry, is suppressed). For $n \geq 3$ the situation becomes more complicated, because $\mathcal{P}_n$ is neither polyhedral nor smooth: any matrix of rank less than $n-1$ is on the boundary, but the boundary is not differentiable at that point.

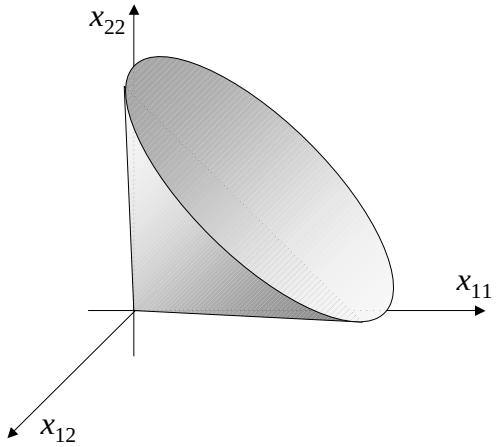

Figure 1: The semidefinite cone for $n = 2$.

The polar cone of $\mathcal{P}$ is itself; in other words,

Proposition 1.5 *A matrix A is positive semidefinite iff $A \cdot B \geq 0$ for every positive semidefinite matrix B.*

1.3 Cross product

This construction probably familiar from physics. For $a, b \in \mathbb{R}^3$, we define their *cross product* as the vector

$$a \times b = |a| \cdot |b| \cdot \sin\phi \cdot u, \tag{1}$$

where ϕ is the angle between a and b ($0 \leq \phi \leq \pi$), and u is a unit vector in $\mathbb{R}^3$ orthogonal to the plane of a and b, so that the triple (a, b, u) is right-handed (positively oriented). The definition of u is ambiguous if $a$and b are parallel, but then $\sin\phi = 0$, so the cross product is 0 anyway. The length of the cross product gives the area of the parallelogram spanned by a and b.

The cross product is distributive with respect to linear combination of vectors, it is anticommutative: $a \times b = -b \times a$, and $a \times b = 0$ if and only if a and b are parallel. The cross product is not associative; instead, it satisfies the identity

$$(a \times b) \times c = (a \cdot c)b - (b \cdot c)a, \tag{2}$$

which implies the *Jacobi Identity*

$$(a \times b) \times c + (b \times c) \times a + (c \times a) \times b = 0. \tag{3}$$

Another useful replacement for the associativity is the following.

$$(a \times b) \cdot c = a \cdot (b \times c) = \det(a, b, c) \tag{4}$$

(here (a, b, c) is the 3×3 matrix with columns a, b and c.

We often use the cross product in the special case when the vectors lie in a fixed plane Π. Let k be a unit vector normal to Π, then $a \times b$ is Ak, where A is the signed area of the parallelogram spanned by a and b (this means that T is positive iff a positive rotation takes the direction of a to the direction of b, when viewed from the direction of k). Thus in this case all the information about $a \times b$ is contained in this scalar A, which in tensor algebra would be denoted by $a \wedge b$. But not to complicate notation, we'll use the cross product in this case as well.

2 Eigenvalues of graphs

2.1 Matrices associated with graphs

We introduce the adjacency matrix, the Laplacian and the transition matrix of the random walk, and their eigenvalues.

Let G be a (finite, undirected, simple) graph with node set $V(G) = \{1, \ldots, n\}$. The *adjacency matrix* of G is be defined as the $n \times n$ matrix $A_G = (A_{ij})$ in which

$$A_{ij} = \begin{cases} 1, & \text{if } i \text{ and } j \text{ are adjacent,} \\ 0, & \text{otherwise.} \end{cases}$$

We can extend this definition to the case when G has multiple edges: we just let A_{ij} be the number of edges connecting i and j. We can also have weights on the edges, in which case we let A_{ij} be the weight of the edges. We could also allow loops and include this information in the diagonal, but we don't need this in this course.

The *Laplacian* of the graph is defined as the $n \times n$ matrix $L_G = (L_{ij})$ in which

$$L_{ij} = \begin{cases} d_i, & \text{if } i = j, \\ -A_{ij}, & \text{if } i \neq j. \end{cases}$$

Here d_i denotes the degree of node i. In the case of weighted graphs, we define $d_i = \sum_j A_{ij}$. So $L_G = D_G - A_G$, where D_G is the diagonal matrix of the degrees of G.

The *transition matrix of the random walk on* G is defined as the $n \times n$ matrix $P_G = (P_{ij})$ in which

$$P_{ij} = \frac{1}{d_i} A_{ij}.$$

So $P_G = D_G^{-1} A$.

The matrices A_G and L_G are symmetric, so their eigenvalues are real. The matrix P_G is not symmetric, but it is conjugate to a symmetric matrix. Let

$$N_G = D_G^{-1/2} A_G D_G^{-1/2},$$

then N_G is symmetric, and

$$P_G = D_G^{-1/2} N_G D_G^{1/2}.$$

The matrices A_G and L_G and N_G are symmetric, so their eigenvalues are real. The matrices P_G and N_G have the same eigenvalues, and so all eigenvalues of P_G are real. We denote these eigenvalues as follows:

$$\begin{aligned} A_G:&\ \lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_n,\\ L_G:&\ \mu_1 \leq \mu_2 \leq \cdots \leq \mu_n,\\ A_G:&\ \nu_1 \geq \nu_2 \geq \cdots \geq \nu_n, \end{aligned}$$

Exercise 2.1 Compute the spectrum of complete graphs, cubes, stars, paths.

We'll often use the (generally non-square) *incidence matrix* of G. This notion comes in two flavors. Let $V(G) = \{1, \ldots, n\}$ and $E(G) = \{e_1, \ldots, e_m$, and let B_G denote the $n \times m$ matrix for which

$$(B_G)_{ij} = \begin{cases} 1 & \text{if } i \text{ is and endpoint of } e_j,\\ 0 & \text{otherwise.} \end{cases}$$

Often, however, the following matrix is more useful: Let us fix an orientation of each edge, to get an oriented graph $\overrightarrow{G}$. Then let $B_{\overrightarrow{G}}$ denote the $n \times m$ matrix for which

$$(B_{\overrightarrow{G}})_{ij} = \begin{cases} 1 & \text{if } i \text{ is the head of } e_j,\\ -1 & \text{if } i \text{ is the tail of } e_j,\\ 0 & \text{otherwise.} \end{cases}$$

Changing the orientation only means scaling some columns by -1, which often does not matter much. For example, it is easy to check that independently of the orientation,

$$L_G = B_{\overrightarrow{G}} B_{\overrightarrow{G}}^{\mathsf{T}}. \tag{5}$$

It is worth while to express this equation in terms of quadratic forms:

$$x^{\mathsf{T}} L_G x = \sum_{ij \in E(G)} (x_i - x_j)^2. \tag{6}$$

2.2 The largest eigenvalue

2.2.1 Adjacency matrix

The Perron–Frobenius Theorem implies immediately that if G is connected, then the largest eigenvalue $\lambda_{\max}$ of A_G of A_G has multiplicity 1. This eigenvalue is relatively uninteresting, it is a kind of "average degree". More precisely, let $d_{\min}$ denote the minimum degree of G, let $\overline{d}$ be the average degree, and let $d_{\max}$ be the maximum degree.

Proposition 2.1 *For every graph G,*

$$\max\{\overline{d}, \sqrt{d_{\max}}\} \leq \lambda_{\max} \leq d_{\max}.$$

Proof.

□

Exercise 2.2 Compute the largest eigenvalue of a star.

2.2.2 Laplacian

For the Laplacian L_G, this corresponds to the smallest eigenvalue, which is really uninteresting, since it is 0:

Proposition 2.2 *The Laplacian L_G is singular and positive semidefinite.*

Proof. The proof follows immediately from (5) or (6), which show that L_G is positive semidefinite. Since $\mathbf{1} = (1, \ldots, 1)^\mathsf{T}$ is in the null space of L_G, it is singular. □

If G is connected, then 0, as an eigenvalue of L_G, has multiplicity 1; we get this by applying the Perron–Frobenius Theorem to $cI - L_G$, where c is a large real number. The eigenvector belonging to this eigenvalue is $\mathbf{1} = (1, \ldots, 1)^\mathsf{T}$ (and its scalar multiples).

We note that for a general graph, the multiplicity of the 0 eigenvalue of the Laplacian is equal to the number of connected components. Similar statement is not true for the adjacency matrix (if the largest eigenvalues of the connected components of G are different, then the largest eigenvalue of the whole graph has multiplicity 1). This illustrates the phenomenon that the Laplacian is often better behaved algebraically than the adjacency matrix.

2.2.3 Transition matrix

The largest eigenvalue of P_G is 1, and it has multiplicity 1 for connected graphs. It is straightforward to check that the right eigenvector belonging to it is $\mathbf{1}$, and the left eigenvector is given by $\pi_i = d_i/(2m)$ (where m is the number of edges). This vector π describes the *stationary distribution* of a random walk, and it is very important in the theory of random walks (see later).

2.3 The smallest eigenvalue

Proposition 2.3 (a) *A graph is bipartite if and only if its spectrum is symmetric about the origin.*

(b) *A connected graph G is bipartite if and only if $\lambda_{\min}(G) = -\lambda_{\max}(G)$.*

Proof.

□

The "only if" part of Proposition 2.3 can be generalized: The ratio between the largest and smallest eigenvalue can be used to estimate the chromatic number (Hoffman [92]).

Theorem 2.4

$$\chi(G) \geq 1 + \frac{\lambda_{\min}}{\lambda_{\max}}.$$

Proof. Let $k = \chi(G)$, then A_G can be partitioned as

$$\begin{pmatrix} 0 & M_{12} & \ldots & M_{1k} \\ M_{21} & 0 & & M_{2k} \\ \vdots & \vdots & \ddots & \\ M_{k1} & M_{k2} & & 0, \end{pmatrix}$$

where M_{ij} is an $m_i \times m_j$ matrix (where m_i is the number of points with color i).

Let $\mathbf{v}$ be an eigenvector belonging to λ_1. Let us break $\mathbf{v}$ into pieces $\mathbf{v}_1, \ldots, \mathbf{v}_k$ of length $m_1, \ldots, m_k$, respectively. Set

$$\mathbf{w}_i = \begin{pmatrix} |\mathbf{v}_i| \\ 0 \\ \vdots \\ 0 \end{pmatrix} \in \mathbb{R}^{m_i} \quad \mathbf{w} = \begin{pmatrix} \mathbf{w}_1 \\ \vdots \\ \mathbf{w}_k \end{pmatrix}.$$

Let B_i be any orthogonal matrix such that

$$B_i \mathbf{w}_i = \mathbf{v}_i \qquad (i = 1, \ldots, k),$$

and

$$B = \begin{pmatrix} B_1 & & & 0 \\ & B_2 & & \\ & & \ddots & \\ 0 & & & B_k \end{pmatrix}.$$

Then $B\mathbf{w} = \mathbf{v}$ and

$$B^{-1}AB\mathbf{w} = B^{-1}A\mathbf{v} = \lambda_1 B^{-1}\mathbf{v} = \lambda_1 \mathbf{w}$$

so $\mathbf{w}$ is an eigenvector of $B^{-1}AB$. Moreover, $B^{-1}AB$ has the form

$$\begin{pmatrix} 0 & B_1^{-1}A_{12}B_2 & \ldots & B_1^{-1}A_{1k}B_k \\ B_2^{-1}A_{21}B_1 & 0 & & B_2^{-1}A_{2k}B_k \\ \vdots & & \ddots & \vdots \\ B_k^{-1}A_{k1}B_1 & B_k^{-1}A_{k2}B_2 & \ldots & 0 \end{pmatrix}.$$

Pick the entry in the upper left corner of each of the k^2 submatrices $B_i^{-1}A_{ij}B_j$ ($A_{ii} = 0$), these form a $k \times k$ submatrix D. Observe that

$$\mathbf{u} = \begin{pmatrix} |\mathbf{v}_1| \\ \vdots \\ |\mathbf{v}_k| \end{pmatrix}$$

is an eigenvector of D; for $\mathbf{w}$ is an eigenvector of $B^{-1}AB$ and has 0 entries on places corresponding to those rows and columns of $B^{-1}AB$, which are to be deleted to get D. Moreover, the eigenvalue belonging to $\mathbf{u}$ is λ_1.

Let $\alpha_1 \geq \cdots \geq \alpha_k$ be the eigenvalues of D. Since D has 0's in its main diagonal,

$$\alpha_1 + \cdots + \alpha_k = 0.$$

On the other hand, λ_1 is an eigenvalue of D and so

$$\lambda_1 \leq \alpha_1,$$

while by the Interlacing Eigenvalue Theorem

$$\lambda_n \leq \alpha_k, \ldots, \lambda_{n-k+2} \leq \alpha_2.$$

Thus

$$\lambda_n + \cdots + \lambda_{n-k+2} \le \alpha_k + \cdots + \alpha_2 = -\alpha_1 \le -\lambda_1.$$

□

Remark 2.5 The proof did not use that the edges were represented by the number 1, only that the non-edges and diagonal entries were 0. So if we want to get the strongest possible lower bound on the chromatic number that this method provides, we can try to find a way of choosing the entries in A corresponding to edges of G in such a way that the right hand side is minimized. This can be done efficiently.

The smallest eigenvalue is closely related to the characterization of linegraphs. The correspondence is not perfect though. To state the result, we need some definitions. Let G be a simple graph. A *pending star* in G is a maximal set of edges which are incident with the same node and whose other endpoints have degree 1. The *linegraph* $L(G)$ of G is defined on $V(L(G)) = E(G)$, where to edges of G are adjacent in $L(G)$ if and only if they have a node in common. A graph H is called a *modified linegraph* of G if it is obtained from $L(G)$ by deleting a set of disjoint edges from each clique corresponding to a pending star of G.

Part (a) of the following theorem is due to Hoffman [91], part (b), to Cameron, Goethals, Seidel and Shult [33].

Proposition 2.6 (a) *Let H be the generalized linegraph of G. Then $\lambda_{\min}(H) \ge -2$; if $|E(G)| > |V(G)|$, then $\lambda_{\min}(H) = -2$.*

(b) *Let H be a simple graph such that $\lambda_{\min}(H) \ge -2$. Assume that $|V(H)| \ge 37$. Then G is a modified linegraph.*

Proof. We only give the proof for part (a), and only in the case when $H = L(G)$. It is easy to check that we have

$$A_{L(G)} = B_G^{\mathsf{T}} B_G - 2I.$$

Since $B_G^T B_G$ is positive semidefinite, all of its eigenvalues are non-negative. Hence, the eigenvalues of $A_{L(G)}$ are ≥ -2. Moreover, if $|V(G)| < |E(G)|$, then

$$r(B^T B) = r(B) \le |V(G)| < |E(G)|$$

($r(X)$ is the rank of the matrix X). So, $B^T B$ has at least one 0 eigenvalue, i.e. $A_{L(G)}$ has at least one -2 eigenvalue. □

Exercise 2.3 Modify the proof above to get (a) in general.

2.4 The eigenvalue gap

The gap between the second and the first eigenvalues is an extremely important parameter in many branches of mathematics.

If the graph is connected, then the largest eigenvalue of the adjacency matrix as well as the smallest eigenvalue of the Laplacian have multiplicity 1. We can expect that the gap between this and the nearest eigenvalue is related to some kind of connectivity measure of the graph.

Indeed, fundamental results due to Alon–Milman [8], Alon [5] and Jerrum–Sinclair [97] relate the eigenvalue gap to expansion (isoperimetric) properties of graphs. These results can be considered as discrete analogues of Cheeger's inequality in differential geometry.

There are many related (but not equivalent) versions of these results. We illustrate this connection by two versions that are of special interest: a spectral characterization of expanders and a bound on the mixing time of random walks on graphs. For this, we discuss very briefly expanders and also random walks and their connections with eigenvalues (see [1] and [129] for more).

The multiplicity of the second largest eigenvalue will be discussed in connection with the Colin de Verdière number.

2.4.1 Expanders

An *expander* is a regular graph with small degree in which the number of neighbors of any set containing at most half of the nodes is at least a constant factor of its size. To be precise, an ε-expander is a graph $G = (V, E)$ in which for every set $S \subset V$ with $|S| \leq |V|/2$, the number of nodes in $V \setminus S$ adjacent to some node in S is at least $\varepsilon|S|$.

Expanders play an important role in many applications of graph theory, in particular in computer science. The most important expanders are d-regular expanders, where $d \geq 3$ is a small constant. Such graphs are not easy to construct. One method is to do a random construction: for example, we can pick d random perfect matchings on $2n$ nodes (independently, uniformly over all perfect matchings), and let G be the union of them. Then a moderately complicated computation shows that G is an ε-expander with positive probability for a sufficiently small ε. Deterministic constructions are much more difficult to obtain; the first construction was found by Margulis [132]; see also [130]. Most of these constructions are based on deep algebraic facts.

Our goal here is to state and prove a spectral characterization of expanders, due to Alon [5], which plays an important role in analyzing some of the above mentioned algebraic constructions. note that since we are considering only regular graphs, the adjacency matrix, the Laplacian and the transition matrix are easily expressed, and so we shall only consider the adjacency matrix.

Theorem 2.7 *Let G be a d-regular graph.*

(a) *If $d - \lambda_2 \geq 2\varepsilon d$, then G is an ε-expander.*

(b) *If G is an ε-expander, then $d - \lambda_2 \geq \varepsilon^2/5$.*

Proof. The proof is similar to the proof of Theorem 2.8 below. □

2.4.2 Edge expansion (conductance)

We study the connection of the eigenvalue gap of the transition matrix with a quantity that can be viewed as an edge-counting version of the expansion. Let $1 = \lambda_1 \geq \lambda_2 \geq \ldots \geq \lambda_n$ be the eigenvalues of P_G.

The *conductance* of a graph $G = (V, E)$ is defined as follows. For two sets $S_1, S_2 \subseteq V$, let $e_G(S_1, S_2)$ denote the number of edges ij with $i \in S_1, j \in S_2$. For every subset $S \subseteq V$, let $d(S) = \sum_{i \in S} d_i$, and define

$$\Phi(G) = \min_{\emptyset \subset S \subset V} \frac{2me_G(S, V \setminus S)}{d(S) \cdot d(V \setminus S)}.$$

For a d-regular graph, this can be written as

$$\Phi(G) = \min_{\emptyset \subset S \subset V} \frac{n}{d} \frac{e_G(S, V \setminus S)}{|S| \cdot |V \setminus S|}.$$

The following basic inequality was proved by Jerrum and Sinclair [97]:

Theorem 2.8 *For every graph G,*

$$\frac{\Phi(G)^2}{16} \leq 1 - \lambda_2 \leq \Phi(G)$$

We start with a lemma expressing the eigenvalue gap of P_G in a manner similar to the Rayleigh quotient.

Lemma 2.9 *For every graph G we have*

$$1 - \lambda_2 = \min \sum_{(i,j) \in E} (x_i - x_j)^2,$$

where the minimum is taken over all vectors $x \in \mathbb{R}^V$ such that

$$\sum_{i \in V} d_i x_i = 0, \qquad \sum_{i \in V} d_i x_i^2 = 1. \tag{7}$$

Proof. As remarked before, the symmetrized matrix $N_G = D_G^{1/2} P_G D_G^{-1/2}$ has the same eigenvalues as P_G. For a symmetric matrix, the second largest eigenvalue can be obtained as

$$\lambda_2 = \max y^{\mathsf{T}} N_G y,$$

where y ranges over all vectors of unit length orthogonal to the eigenvector belonging to the largest eigenvalue. This latter eigenvector is given (up to scaling) by $v_i = \sqrt{d_i}$, so the conditions on y are

$$\sum_{i \in V} \sqrt{d_i} y_i = 0, \qquad \sum_{i \in V} y_i^2 = 1. \tag{8}$$

Let us write $y_i = x_i \sqrt{d_i}$, then the conditions (8) on y translate into conditions (7) on x. Furthermore,

$$\begin{aligned} \sum_{(i,j) \in E} (x_i - x_j)^2 &= 2m \sum_{(i,j) \in E} (\frac{y_i}{\sqrt{d_i}} - \frac{y_j}{\sqrt{d_j}})^2 \\ &= \sum_i d_i \frac{y_i^2}{d_i} - 2 \sum_{(i,j) \in E} (\frac{y_i y_j}{\sqrt{d_i}\sqrt{d_j}} \\ &= 1 - y^{\mathsf{T}} N_G y. \end{aligned}$$

The minimum of the left hand side subject to (7) is equal to the minimum of the right hand side subject to (8), which proves the Lemma. □

Now we can prove the theorem.

Proof. The upper bound is easy: let $\emptyset \neq S \subset V$ be a set with

$$\frac{2me_G(S, V \setminus S)}{d(S) \cdot d(V \setminus S)} = \Phi(G).$$

Let x be a vector on the nodes defined by

$$x_i = \begin{cases} \sqrt{\frac{d(V \setminus S)}{2md(S)}} & \text{if } i \in S, \\ -\sqrt{\frac{d(S)}{2md(V \setminus S)}} & \text{if } i \in V \setminus S. \end{cases}$$

It is easy to check that

$$\sum_{i \in V} d_i x_i = 0, \qquad \sum_{i \in V} d_i x_i^2 = 1.$$

Thus by Lemma 2.9,

$$\begin{aligned} 1 - \lambda_2 &\geq \sum_{ij \in E} (x_i - x_j)^2 = e_G(S, V \setminus S) \left(\sqrt{\frac{d(V \setminus S)}{2md(S)}} + \sqrt{\frac{d(S)}{2md(V \setminus S)}} \right)^2 \\ &= \frac{2me_G(S, V \setminus S)}{d(S)d(V \setminus S)} = \Phi(G). \end{aligned}$$

It is easy to see that the statement giving the lower bound can be written as follows: let $y \in \mathbb{R}^V$ and let $\hat{y} = (1/2m) \sum_i d_i y_i$. Then we have

$$\sum_{(i,j) \in E} (y_i - y_j)^2 \geq \frac{\Phi^2}{16} \sum_i (y_i - \hat{y})^2. \tag{9}$$

To prove this, we need a lemma that can be thought of as a linear version of (9). For every real vector $y = (y_1, \ldots, y_n)$, we define its *median* (relative to the degree sequence d_i) as a the member y_M of the sequence for which

$$\sum_{k:\, y_k \leq y_M} d_k \leq m, \qquad \sum_{k:\, y_k > y_M} d_k < m.$$

Lemma 2.10 *Let $G = (V, E)$ be a graph with conductance $\Phi(G)$. Let $y \in \mathbb{R}^V$, and let y_M be the median of y. Then*

$$\sum_{(i,j) \in E} |y_i - y_j| \geq \frac{\Phi}{2} \sum_i d_i |y_i - y_M|.$$

Proof. [of the Lemma] We may label the nodes so that $y_1 \leq y_2 \leq \ldots \leq y_n$. We also may assume that $y_M = 0$ (the assertion of the Lemma is invariant under shifting the entries of y). Substituting

$$y_j - y_i = (y_{i+1} - y_i) + \cdots + (y_j - y_{j-1}),$$

we have

$$\sum_{(i,j) \in E} |y_i - y_j| = \sum_{k=1}^{n-1} e(\leq k, > k)(y_{k+1} - y_k).$$

By the definition of Φ, this implies

$$\begin{aligned}\sum_{(i,j)\in E} |y_i - y_j| &\geq \frac{\Phi}{2m} \sum_{k=1}^{n-1} d(\leq k) d(> k)(y_{k+1} - y_k) \\ &\geq \frac{\Phi}{2m} \sum_{k<M} d(\leq k) m (y_{k+1} - y_k) + \frac{\Phi}{2m} \sum_{k\geq M} m d(> k)(y_{k+1} - y_k) \\ &= \frac{\Phi}{2} \sum_{i\leq M} d_i y_i - \frac{\Phi}{2} \sum_{i>M} d_i y_i \\ &= \frac{\Phi}{2} \sum_i d_i |y_i|.\end{aligned}$$

□

Now we return to the proof of the lower bound in Theorem 2.8. Let x be a unit length eigenvector belonging to λ_2. We may assume that the nodes are labeled so that $x_1 \geq x_2 \geq \ldots \geq x_n$. Let x_M be the median of x. Note that the average $(1/(2m)) \sum_i d_i x_i = 0$. Set $z_i = \big(\max\{0, x_i - x_M\}\big)$ and $u_i = \big(\max\{0, x_M - x_i\}\big)$. Then

$$\sum_i d_i z_i^2 + \sum_i d_i u_i^2 = \sum_i d_i (x_i - x_M)^2 = \sum_i x_i^2 + 2m x_M^2 \geq \sum_i d_i x_i^2 = 1,$$

and so we may assume (replacing x by $-x$ if necessary) that

$$\sum_i d_i z_i^2 \geq \frac{1}{2}.$$

By Lemma 2.10

$$\sum_{(i,j)\in E} |z_i^2 - z_j^2| \geq \frac{\Phi}{2} \sum_i d_i z_i^2.$$

On the other hand, using the Cauchy-Schwartz inequality,

$$\begin{aligned}\sum_{(i,j)\in E} |z_i^2 - z_j^2| &= \sum_{(i,j)\in E} |z_i - z_j| \cdot |z_i + z_j| \\ &\leq \left(\sum_{(i,j)\in E} (z_i - z_j)^2 \right)^{1/2} \left(\sum_{(i,j)\in E} (z_i + z_j)^2 \right)^{1/2}.\end{aligned}$$

Here the second factor can be estimated as follows:

$$\sum_{(i,j)\in E} (z_i + z_j)^2 \leq 2 \sum_{(i,j)\in E} (z_i^2 + z_j^2) = 2 \sum_i d_i z_i^2.$$

Combining these inequalities, we obtain

$$\begin{aligned}\sum_{(i,j)\in E} (z_i - z_j)^2 &\geq \left(\sum_{(i,j)\in E} |z_i^2 - z_j^2| \right)^2 \Big/ \sum_{(i,j)\in E} (z_i + z_j)^2 \\ &\geq \frac{\Phi^2}{4} \left(\sum_i d_i z_i^2 \right)^2 \Big/ 2 \sum_i d_i z_i^2 = \frac{\Phi^2}{8} \sum_i d_i z_i^2 \geq \frac{\Phi^2}{16}.\end{aligned}$$

Since

$$\sum_{(i,j)\in E} (x_i - x_j)^2 \geq \sum_{(i,j)\in E} (z_i - z_j)^2,$$

from here we can conclude by Lemma 2.9. □

The quantity $\Phi(G)$ is NP-complete to compute. An important theorem of Leighton and Rao gives an approximate min-max theorem for it, which also yields a polynomial time approximation algorithm, all with an error factor of $O(\log n)$.

2.4.3 Random walks

A *random walk* on a graph G is a random sequence $(v^0, v^1, \dots)$ of nodes constructed as follows: We pick a starting point v^0 from a specified initial distribution σ, we select a neighbor v^1 of it at random (each neighbor is selected with the same probability $1/d(v^0)$), then we select a neighbor v^2 of this node v^1 at random, etc. We denote by σ^k the distribution of v^k.

In the language of probability theory, a random walk is a finite time-reversible Markov chain. (There is not much difference between the theory of random walks on graphs and the theory of finite Markov chains; every Markov chain can be viewed as random walk on a directed graph, if we allow weighted edges, and every time-reversible Markov chain can be viewed as random walks on an edge-weighted undirected graph.)

Let π denote the probability distribution in which the probability of a node is proportional to its degree:

$$\pi(v) = \frac{d(v)}{2m}.$$

This distribution is called the *stationary distribution* of the random walk. It is easy to check that if v^0 is selected from π, then after any number of steps, v^k will have the same distribution π. This explains the name of π. Algebraically, this means that π is a left eigenvector of P_G with eigenvalue 1:

$$\pi^T P_G = \pi^T.$$

Theorem 2.11 *If G is a connected nonbipartite graph, then $\sigma^k \to \pi$ for every starting distribution σ.*

It is clear that the conditions are necessary.

Before proving this theorem, let us make some remarks on one of its important applications, namely *sampling*. Suppose that we want to pick a random element uniformly from some finite set. We can then construct a connected nonbipartite regular graph on this set, and start a random walk on this graph. A node of the random walk after sufficiently many steps is therefore essentially uniformly distributed.

(It is perhaps surprising that there is any need for a non-trivial way of generating an element from such a simple distribution as the uniform. But think of the first application of random walk techniques in real world, namely shuffling a deck of cards, as generating a random permutation of 52 elements from the uniform distribution over all permutations. The problem is that the set we want a random element from is exponentially large. In many applications, it has in addition a complicated structure; say, we consider the set of lattice points in a convex body or the set of linear extensions of a partial order. Very often this random walk sampling is the only known method.)

With this application in mind, we see that not only the fact of convergence matters, but also the rate of this convergence, called the *mixing rate*. The proof below will show how this relates to the eigenvalue gap. In fact, we prove:

Theorem 2.12 *Let $\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_n$ be the eigenvalues of P_G, and let $\mu = \max\{\lambda_2, \lambda_n\}$. Then for every starting node i and any node j, and every $t \geq 0$, we have*

$$|\Pr(v^t = j) - \pi(j)| \leq \sqrt{\frac{\pi(j)}{\pi(i)}}\mu^t.$$

More generally, for every set $A \subseteq V$,

$$|\Pr(v^t \in A) - \pi(A)| \leq \sqrt{\frac{\pi(A)}{\pi(i)}}\mu^t.$$

Proof. We prove the first inequality; the second is left to the reader as an exercise. We know that the matrix N_G has the same eigenvalues as P_G, and it is symmetric, so we can write it as

$$N_G = \sum_{k=1}^{n} \lambda_k v_k v_k^{\mathsf{T}},$$

where $v_1, \ldots, v_n$ are mutually orthogonal eigenvectors. It is easy to check that we can choose

$$v_{1i} = \sqrt{\pi_i}$$

(we don't know anything special about the other eigenvectors). Hence we get

$$\begin{aligned}\Pr(v^t = j) = (P^t)_{ij} = e_i^{\mathsf{T}} D^{-1/2} N^t d^{1/2} e_j = \sum_{k=1}^{n} \lambda_k^t (e_i^{\mathsf{T}} D^{-1/2} v_k)(e_j^{\mathsf{T}} D^{1/2} v_k) \\ = \sum_{k=1}^{n} \lambda_k^t \frac{1}{\sqrt{\pi(i)}} v_{ki} \sqrt{\pi(j)} v_{kj} = \pi(j) + \sqrt{\frac{\pi(j)}{\pi(i)}} \sum_{k=2}^{n} \lambda_k^t v_{ki} v_{kj}.\end{aligned}$$

Here the first term is the limit; we need to estimate the second. We have

$$\Big|\sum_{k=2}^{n} \lambda_k^t v_{ki} v_{kj}\Big| \leq \mu^t \sum_{k=2}^{n} \Big|v_{ki} v_{kj}\Big| \leq \mu^t \sum_{k=1}^{n} \Big|v_{ki} v_{kj}\Big| \leq \mu^t \left(\sum_{k=1}^{n} v_{ki}^2\right)^{1/2} \left(v_{kj}^2\right)^{1/2} = \mu^t.$$

This proves the inequality. □

If we want to find a bound on the number of steps we need before, say,

$$|\Pr(v^k \in A) - \pi(A)| < \varepsilon$$

holds for every j, then it suffices to find a k for which

$$\mu^k < \varepsilon\sqrt{\pi_i}.$$

Writing $mu = 1 - \gamma$, and using that $1 - \gamma < e^{-\gamma}$, it suffices to have

$$e^{-\gamma k} < \varepsilon\sqrt{\pi_i},$$

and expressing k,

$$k > \frac{1}{\gamma}\Big(\ln\frac{1}{\varepsilon} + \frac{1}{2}\ln\frac{1}{\pi_i}\Big)$$

So we see that (up to logarithmic factors), it is the reciprocal of the eigenvalue gap that governs the mixing time.

In applications, the appearance of the smallest eigenvalue λ_n is usually not important, and what we need to work on is bounding the *eigenvalue gap* $1 - \lambda_2$. The trick is the following: If the smallest eigenvalue is too small, then we can modify the walk as follows. At each step, we flip a coin and move with probability $1/2$ and stay where we are with probability $1/2$. The stationary distribution of this modified walk is the same, and the transition matrix P_G is replaced by $\frac{1}{2}(P_G + I)$. For this modified walk, all eigenvalues are nonnegative, and the eigenvalue gap is half of the original. So applying the theorem to this, we only use a factor of 2.

Explanation of conductance: In a stationary random walk on G, we cross every edge in every direction with the same frequency, once in every $2m$ steps on the average. So $Q(S, V \setminus S)$ is the frequency with which we step out from S. If instead we consider a sequence of independent samples from π, the frequency with which we step out from S is $\pi(S)\pi(V \setminus S)$. The ratio of these two frequencies is one of many possible ways comparing a random walk with a sequence of independent samples.

Exercise 2.4 Let $G = (V, E)$ be a simple graph, and define

$$\rho(G) = \min_{\emptyset \subset S \subset V} \frac{e_G(S, V \setminus S)}{|S| \cdot |V \setminus S|}.$$

Let λ_2 denote the second smallest eigenvalue of the Laplacian L_G of a graph G. Then

$$\lambda_2 \le n\rho(G) \le \sqrt{\lambda_2 d_{\max}}.$$

2.5 The number of different eigenvalues

Multiplicity of eigenvalues usually corresponds to symmetries in the graph (although the correspondence is not exact). We prove two results in this direction. The following theorem was proved by Mowshowitz [141] and Sachs [159]:

Theorem 2.13 *If all eigenvalues of A are different, then every automorphism of A has order 1 or 2.*

Proof. Every automorphism of G can be described by a permutation matrix P such that $AP = PA$. Let u be an eigenvector of A with eigenvalue λ. Then

$$A(Pu) = PAu = P(\lambda u) = \lambda(Pu),$$

so Pu is also an eigenvector of A with the same eigenvalue. Since Pu has the same length as u, it follows that $Pu = \pm u$ and hence $P^2u = u$. This holds for every eigenvector u of A, and since there is a basis consisting of eigenvectors, it follows that $P^2 = I$. □

A graph G is called *strongly regular*, if it is regular, and there are two nonnegative integers a and b such that for every pair i, j of nodes the number of common neighbors of i and j is

$$\begin{cases} a, & \text{if } a \text{ and } b \text{ are adjacent,} \\ b, & \text{if } a \text{ and } b \text{ are nonadjacent.} \end{cases}$$

Example 2.14 Compute the spectrum of the Petersen graph, Paley graphs, incidence graphs of finite projective planes.

The following characterization of strongly regular graphs is easy to prove:

Theorem 2.15 *A connected graph G is strongly regular if and only if it is regular and A_G has at most 3 different eigenvalues.*

Proof. The adjacency matrix of a strongly regular graph satisfies

$$A^2 = aA + b(J - A - I) + dI. \tag{10}$$

The largest eigenvalue is d, all the others are roots of the equation

$$\lambda^2 - (a-b)\lambda - (d-b), \tag{11}$$

Thus there are at most three distinct eigenvalues.

Conversely, suppose that G is d-regular and has at most three different eigenvalues. One of these is d, with eigenvector $\mathbf{1}$. Let λ_1 and λ_2 be the other two (I suppose there are two more—the case when there is at most one other is easy). Then

$$B = A^2 - (\lambda_1 + \lambda_2)A + \lambda_1\lambda_2 I$$

is a matrix for which $Bu = 0$ for every eigenvector of A except $\mathbf{1}$ (and its scalar multiples). Furthermore, $B\mathbf{1} = c\mathbf{1}$, where $c = (d-\lambda_1)(d-\lambda_2)$. Hence $B = (c/n)J$, and so

$$A^2 = (\lambda_1 + \lambda_2)A - \lambda_1\lambda_2 I + (c/n)J.$$

This means that $(A^2)_{ij}$ $(i \neq j)$ depends only on whether i and j are adjacent, proving that G is strongly regular. □

We can get more out of equation (11). We can solve it:

$$\lambda_{1,2} = \frac{a - b \pm \sqrt{(a-b)^2 + 4(d-b)}}{2}. \tag{12}$$

Counting induced paths of length 2, we also get the equation

$$(d - a - 1)d = (n - d - 1)b. \tag{13}$$

Let m_1 and m_2 be the multiplicities of the eigenvalues λ_1 and λ_2. Clearly

$$m_1 + m_2 = n - 1 \tag{14}$$

Taking the trace of A, we get

$$d + m_1\lambda_1 + m_2\lambda_2 = 0,$$

or

$$2d + (n-1)(a-b) + (m_1 - m_2)\sqrt{(a-b)^2 + 4(d-b)} = 0. \tag{15}$$

If the square root is irrational, the only solution is $d = (n-1)/2$, $b = (n-1)/4$, $a = b-1$. There are many solutions where the square root is an integer.

A nice application of these formulas is the "Friendship Theorem":

Theorem 2.16 *If G is a graph in which every two nodes have exactly one common neighbor, then it has a node adjacent to every other node.*

Proof. First we show that two non-adjacent nodes must have the same degree. Suppose that there are two non-adjacent nodes u, v of different degree. For every neighbor w of u there is a common neighbor w' of w and v. For different neighbors w_1 and w_2 of u, the nodes w_1' and w_2' must be different, else $w-1$ and $w-2$ would have two common neighbors. So v has at least as many neighbors as u. By a symmetric reasoning, we get $d_u = d_v$.

If G has a node v whose degree occurs only once, then by the above, v must be connected to every other node, and we are done. So suppose that no such node exists.

If G has two nodes u and v of different degree, then it contains two other nodes x and y such that $d_u = d_x$ and $d_v = d_y$. But then both x and u are common neighbors of v and y, contradicting the assumption.

Now if G is regular, then it is strongly regular, and $a = b = 1$. From (15),

$$d + (m_1 - m_2)\sqrt{d-1} = 0.$$

The square root must be integral, hence $d = k^2 + 1$. But then $k \mid k^2 + 1$, whence $k = 1$, $d = 2$, and the graph is a triangle, which is not a counterexample. □

Exercise 2.5 Prove that every graph with only two different eigenvalues is complete.

Exercise 2.6 Describe all disconnected strongly regular graphs. Show that there are disconnected graphs with only 3 distinct eigenvalues that are not strongly regular.

2.6 Spectra of graphs and optimization

There are many useful connections between the eigenvalues of a graph and its combinatorial properties. The first of these follows easily from interlacing eigenvalues.

Proposition 2.17 *The maximum size $\omega(G)$ of a clique in G is at most $\lambda_1 + 1$. This bound remains valid even if we replace the non-diagonal 0's in the adjacency matrix by arbitrary real numbers.*

The following bound on the chromatic number is due to Hoffman.

Proposition 2.18 *The chromatic number $\chi(G)$ of G is at least $1-(\lambda_1/\lambda_n)$. This bound remains valid even if we replace the 1's in the adjacency matrix by arbitrary real numbers.*

The following bound on the maximum size of a cut is due to Delorme and Poljak [45, 44, 139, 147], and was the basis for the Goemans-Williamson algorithm discussed in the introduction.

Proposition 2.19 *The maximum size $\gamma(G)$ of a cut in G is at most $|E|/2 - (n/4)\lambda_n$. This bound remains valid even if we replace the diagonal 0's in the adjacency matrix by arbitrary real numbers.*

Observation: to determine the best choice of the "free" entries in 2.17, 2.18 and 2.19 takes a semidefinite program. Consider 2.17 for example: we fix the diagonal entries at 0, the entries corresponding to edges at 1, but are free to choose the entries corresponding to non-adjacent

pairs of vertices (replacing the off-diagonal 1's in the adjacency matrix). We want to minimize the largest eigenvalue. This can be written as a semidefinite program:

$$\begin{array}{ll} \text{minimize} & t \\ \text{subject to} & tI - X \succeq 0, \\ & X_{ii} = 0 \quad (\forall i \in V), \\ & X_{ij} = 1 \quad (\forall ij \in E). \end{array}$$

It turns out that the semidefinite program constructed for 2.18 is just the dual of this, and their common optimum value is the parameter $\vartheta(G)$ introduced before. The program for 2.19 gives the approximation used by Goemans and Williamson (for the case when all weights are 1, from which it is easily extended).

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