Background material

Geometric Graph Theory
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1.1 Background from linear algebra

1.1.1 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 1.1.1 (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 1.1.2 (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.*

1.1.2 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 1.1.3 *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 $\text{tr}(A) = 0$ 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 1.1.4 *If A and B are positive semidefinite matrices, then $\text{tr}(AB) \geq 0$, 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

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

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

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

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 $n \ge 2$; for $n = 2$ it is a nice rotational cone (Figure 1.1; the fourth coordinate x_{21}, which is always equal to x_{12} by symmetry, is suppressed). For $n \ge 3$ 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.

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

Proposition 1.1.5 *A matrix A is positive semidefinite iff $A \cdot B \ge 0$ for every positive semidefinite matrix B.*

1.1.3 Cross product

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

$$a \times b = |a| \cdot |b| \cdot \sin\phi \cdot u, \tag{1.1}$$

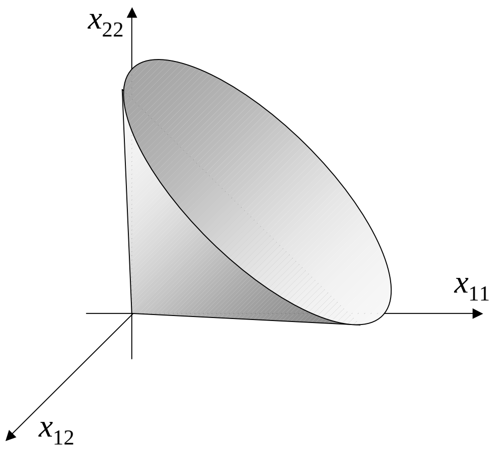

Figure 1.1: The semidefinite cone for $n = 2$.

where ϕ is the angle between a and b ($0 \le \phi \le \pi$), 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

$$(a \times b) \times c = (a \cdot c)b - (b \cdot c)a, \tag{1.2}$$

which implies the *Jacobi Identity*

$$(a \times b) \times c + (b \times c) \times a + (c \times a) \times b = 0. \tag{1.3}$$

Another useful replacement for the associativity is the following.

$$(a \times b) \cdot c = a \cdot (b \times c) = \det(a, b, c) \tag{1.4}$$

(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.

1.2 Eigenvalues of graphs

1.2.1 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 $V(G) = \{1, \dots, n\}$. 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:

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

If more than one graphs are considered, we denote the eigenvalues by $\lambda_1(G)$ etc.

Exercise 1.1 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 $V(G) = \{1, \dots, n\}$ and $E(G) = \{e_1, \dots, e_m$, 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,

$$L_G = B_{\overrightarrow{G}} B_{\overrightarrow{G}}^{\mathsf{T}}. \tag{1.5}$$

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

$$x^{\mathsf{T}} L_G x = \sum_{ij \in E(G)}^{n} (x_i - x_j)^2. \tag{1.6}$$

1.2.2 The largest eigenvalue

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 1.2.1 *Let G' be a subgraph of G. Then*

$$\lambda_1(G) \geq \lambda_1(G').$$

Proposition 1.2.2 *For every graph G,*

$$\max\{\overline{d}, \sqrt{d_{\max}}\} \leq \lambda_1 \leq d_{\max}.$$

Proof. Let $u = (1/\sqrt{n}, \ldots, 1/\sqrt{n})^{\mathsf{T}}$, then

$$\lambda_1 \geq u^{\mathsf{T}} A_G u = \frac{1}{n} \sum_{i,j} A_{ij} = \frac{2m}{n} = \overline{d}.$$

Let H denote the star with $d_{\max}$ rays. Then $H \subseteq G$, and hence by Proposition 1.2.1,

$$\lambda_1(G) \geq \lambda_1(H) = \sqrt{d_{\max}}.$$

Finally, let v_1 denote the eigenvalue belonging to λ_1, and $v_1 = (v_{11}, \ldots, v_{1n})^{\mathsf{T}}$. We may assume that $v_{11} \geq v_{12} \geq \ldots$. Then

$$\lambda_1 v_{11} = \sum_{i=1}^{n} A_{1i} v_{1i} \leq \sum_{i=1}^{n} A_{1i} v_{11} = d_1 v_{11} \leq d_{\max} v_{11},$$

and hence $\lambda_1 \leq d_{\max}$. □

Exercise 1.2 Compute the largest eigenvalue of a star.

Laplacian

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

Proposition 1.2.3 *The Laplacian L_G is singular and positive semidefinite.*

Proof. The proof follows immediately from (1.5) or (1.6), which show that L_G is positive semidefinite. Since $\mathbf{1} = (1, \dots, 1)^\mathsf{T}$ is in the null space of L_G, it is singular. $\square$

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 $\mathbf{1} = (1, \dots, 1)^\mathsf{T}$ (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.

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).

1.2.3 The smallest eigenvalue

Proposition 1.2.4 (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 $\lambda_n = -\lambda_1$.*

Proof. Assume that G is bipartite, with bipartition $V = U \cup W$. For every vector $v \in \mathbb{R}^V$, let $\widetilde{v}$ denote the vector obtained by changing the sign of every coordinate v_i, $i \in W$. Then if v is an eigenvector with eigenvalue λ, then

$$A_G \widetilde{v} = -\lambda v,$$

and so $-\lambda$ is also an eigenvalue with the same multiplicity. This proves the "only if" part of (a) and also of (b).

Assume that G is connected and $\lambda_n(G) = -\lambda_1(G)$. Let v denote an eigenvector of unit length belonging to λ_n. Then

$$|\lambda_n| = \Big|\sum_{i,j} A_{ij} v_i v_j\Big| \le \sum_{i,j} A_{ij} |v_i| \cdot |v_j| \le \lambda_1.$$

It follows that we must have equality throughout. In particular, the vector $v' = (|v_i| : \ i \in V)$ is and eigenvector belonging to λ_1, and hence $|v_i| \neq 0$. Furthermore, $A_{ij} v_i v_j$ must be nonpositive for every i and j, which implies that if i and j are adjacent, then v_i and v_j have different signs.

Hence $U = \{i : v_i > 0\}$ and $W = \{i : v_i < 0\}$ is a bipartition of G. This proves the "if" part of (b).

Finally, assume that the spectrum of G is symmetric with respect to the origin. Let G_1 be a connected component of G which has λ_n as an eigenvalue. Then the largest eigenvalue of G_1 is λ_1,and so by part (b), G_1 is bipartite. Thus the whole spectrum of G_1 is symmetric about 0, and so if we delete G_1, the spectrum of the remaining graph is still symmetric. Proceeding similarly, we conclude that G is bipartite. □

The "only if" part of Proposition 1.2.4 can be generalized: The ratio between the largest and smallest eigenvalue can be used to estimate the chromatic number (Hoffman [92]).

Theorem 1.2.5

$$\chi(G) \geq 1 - \frac{\lambda_1}{\lambda_n}.$$

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

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

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 $\mathbf{v}_1, \dots, \mathbf{v}_k$ of length $m_1, \dots, m_k$, 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

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

and

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

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

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

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

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

□

Remark 1.2.6 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 by semidefinite optimization.

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

(b) *Let H be a simple graph such that $\lambda_{\min}(H) \geq -2$. Assume that $|V(H)| \geq 37$. 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

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

($r(X)$ 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 1.3 Modify the proof above to get (a) in general.

1.2.4 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 is captured by the Colin de Verdière number.

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 1.2.8 *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 1.2.9 below. □

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

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

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 1.2.9 *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 1.2.10 *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

$$\sum_{i \in V} d_i x_i = 0, \qquad \sum_{i \in V} d_i x_i^2 = 1. \tag{1.7}$$

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

$$\sum_{i\in V} \sqrt{d_i} y_i = 0, \qquad \sum_{i\in V} y_i^2 = 1. \tag{1.8}$$

Let us write $y_i = x_i\sqrt{d_i}$, then the conditions (1.8) on y translate into conditions (1.7) 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 (1.7) is equal to the minimum of the right hand side subject to (1.8), 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 1.2.10,

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

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

$$\sum_{(i,j)\in E}(y_i - y_j)^2 \geq \frac{\Phi^2}{16}\sum_i (y_i - \hat{y})^2. \tag{1.9}$$

To prove this, we need a lemma that can be thought of as a linear version of (1.9). For every real vector $y = (y_1, \dots, y_n)$, we define its *median* (relative to the degree sequence d_i) as a the member y_M of the sequence for which

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

Lemma 1.2.11 *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*

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

Proof. [of the Lemma] We may label the nodes so that $y_1 \le y_2 \le \ldots \le y_n$. 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

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

By the definition of Φ, this implies

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

□

Now we return to the proof of the lower bound in Theorem 1.2.9. Let x be a unit length eigenvector belonging to λ_2. We may assume that the nodes are labeled so that $x_1 \ge x_2 \ge \ldots \ge x_n$. 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

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

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

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

By Lemma 1.2.11

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

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 1.2.10. □

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 $O(\log n)$.

1.2.5 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 1.2.12 *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 1.2.13 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 1.2.14 *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

$$A^2 = aA + b(J - A - I) + dI. \tag{1.10}$$

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

$$\lambda^2 - (a - b)\lambda - (d - b), \tag{1.11}$$

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 (1.11). We can solve it:

$$\lambda_{1,2} = \frac{a - b \pm \sqrt{(a - b)^2 + 4(d - b)}}{2}. \tag{1.12}$$

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

$$(d - a - 1)d = (n - d - 1)b. \tag{1.13}$$

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

$$m_1 + m_2 = n - 1 \tag{1.14}$$

Taking the trace of A, we get

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

or

$$2d + (n-1)(a-b) + (m_1 - m_2)\sqrt{(a-b)^2 + 4(d-b)} = 0. \tag{1.15}$$

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 1.2.15 *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 (1.15),

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

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. $\square$

Exercise 1.4 Prove that every graph with only two different eigenvalues is complete.

Exercise 1.5 Describe all disconnected strongly regular graphs. Show that there are disconnected graphs with only 3 distinct eigenvalues that are not strongly regular.

1.2.6 Eigenvectors

Relatively little is known about the eigenvectors belonging to various eigenvalues. For a connected graph, the Perron–Frobenius Theorem implies that the eigenvector belonging to the largest eigenvalue $\lambda_{\max}$ is uniquely determined (up to scaling), and it is all-positive (or all-negative).

For the other eigenvectors, we prove an important lemma of Van der Holst [86] and Colin de Verdière [41].

Lemma 1.2.16 *Let G be a connected graph, let λ be an eigenvalue of A with multiplicity s, and let r be the number of eigenvalues larger than λ. Let x be any eigenvector belonging to λ, and let a, b and c denote the number of connected components of the subgraph spanned by* $\mathrm{supp}_+(x)$, $\mathrm{supp}_-(x)$ *and* $\mathrm{supp}(x)$*, respectively. Then*

(a) $c \leq s$;

(b) $a + b \leq r + c$;

(c) *if* x *has minimal support among the eigenvectors belonging to* λ, *then* $a + b \leq r + 1$.

(d) A *has at least* $a + b$ *eigenvalues* $\geq \lambda$.

Proof. Let $M = \lambda I - A$. Let $H_1, \dots, H_a$ and $H_{a+1}, \dots, H_{a+b}$ be the connected components of the subgraph spanned by $\text{supp}_+(x)$ and $\text{supp}_(x)$, respectively. Let x_i be the restriction of x onto H_i, extended by 0's so that it is a vector in $\mathbb{R}^V$. Thus $x = x_1 + \dots + x_{a+b}$.

For $z \in \mathbb{R}^{a+b}$, let

$$y = \sum_{i=1}^{a+b} z_i x_i. \tag{1.16}$$

Then

$$y^\mathsf{T} M y = \sum_{i,j=1}^{a+b} z_i z_j x_i^\mathsf{T} M x_j = \sum_{i,j=1}^{a+b} W_{ij} z_i z_j = z^\mathsf{T} W z,$$

where $W_{ij} = -x_i^\mathsf{T} M x_j$ and W is the $(a + b) \times (a + b)$ matrix $W = (W_{ij})$. We can observe the following properties:

(i) $W_{ij} = 0$ if there is no edge between H_i and H_j; in particular, if $1 \leq i, j \leq a$ or $a + 1 \leq i, j \leq b$.

(ii) $W_{ij} \geq 0$ for $i \neq j$. It suffices to verify this when $1 \leq i \leq a$ and $a + 1 \leq j \leq b$. But then in $W_{ij} = x_i^\mathsf{T} M x_j$ all non-zero terms are positive.

(iii) $\sum_j W_{ij} = x_i^\mathsf{T} \sum_j M x_j = x_i^\mathsf{T} M x = 0$.

It follows from (iii) that the quadratic form belonging to W can be written as

$$z^\mathsf{T} W z = \sum_{i,j=1}^{a+b} W_{ij} z_i z_j = -\sum_{i<j} W_{ij} (z_i - z_j)^2,$$

and so this form is negative semidefinite. Furthermore, $z^\mathsf{T} W z = 0$ if and only if $z_i = z_j$ whenever there is an edge between the components H_i and H_j; in other words, z is constant on the connected components of $\text{supp}(x)$. So the dimension of the nullspace of W is exactly c. If $Wz = 0$, then for every vector y defined by (1.16) we have $Mz = 0$, so the dimension of the nullspace of M is at least c, which proves (a). Furthermore, $z^\mathsf{T} W z < 0$ on every vector z in the range of W, which has dimension $a+b-c$. So $y^\mathsf{T} M y < 0$ on an $(a+b-c)$-dimensional subspace, and hence M must have at least $a + b - c$ negative eigenvalues, proving (b).

Suppose that x has minimal support among the eigenvectors belonging to λ. Then no vector $z \in \mathbb{R}^{a+b}$ with $Wz = 0$ can have a zero coordinate, since then the corresponding y would be an eigenvector of A belonging to λ with smaller support. Hence the dimension of the nullspace of W is at most 1. From here (c) follows.

(d) is trivial by (a) and (b), since $r + s \geq r + c \geq a + b$. $\square$

1.2.7 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 1.2.17 *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.*

Let us recall Hoffman's bound on the chromatic number, with a supplement.

Proposition 1.2.18 *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.

Proposition 1.2.19 *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 1.2.17, 1.2.18 and 1.2.19 takes a semidefinite program. Consider 1.2.17 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:

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

It turns out that the semidefinite program constructed for 1.2.18 is just the dual of this, and their common optimum value is the parameter $\vartheta(G)$ introduced before. The program for 1.2.19 gives the approximation used by Goemans and Williamson (for the case when all weights are 1, from which it is easily extended).

1.3 Convex polytopes

1.3.1 Polytopes and polyhedra

The convex hull of a finite set of points in $\mathbb{R}^d$ is called a (convex) *polytope*. The intersection of a finite number of halfspaces in $\mathbb{R}^d$ is called a (convex) *polyhedron*.

Proposition 1.3.1 *Every polytope is a polyhedron. A polyhedron is a polytope if and only if it is bounded.*

For every polytope, there is a unique smallest affine subspace that contains it, called its *affine hull*. The *dimension* of a polytope is the dimension of it affine hull. A polytope in $\mathbb{R}^d$ that has dimension d (equivalently, that has an interior point) is called a *d-polytope*.

A hyperplane H is said to *support* the polytope if it has a point in common with the polytope and the polytope is contained in one of the closed halfspaces with boundary H. A *face* of a polytope is its intersection with a supporting hyperplane. A face of a polytope that has dimension one less than the dimension of the polytope is called a *facet*. A face of dimension 0 (i.e., a single point) is called a *vertex*.

Proposition 1.3.2 *Every face of a polytope is a polytope. Every vertex of a face is a vertex of the polytope. Every polytope has a finite number of faces.*

Proposition 1.3.3 *Every polytope is the convex hull of its facets. The set of vertices is the unique minimal finite set of points whose convex hull is the polytope.*

Let P be a d-polytope. Then every facet F of P spans a (unique) supporting hyperplane, and the hyperplane is the boundary of a uniquely determined halfspace that contains the polytope. We'll call this halfspace the *halfspace of* F.

Proposition 1.3.4 *Every polytope is the intersection of the halfspaces of its facets.*

1.3.2 The skeleton of a polytope

The vertices and edges of a polytope P form a simple graph G_P, which we call the *skeleton* of the polytope.

Proposition 1.3.5 *Let P be a polytope in $\mathbb{R}^d$ and $a \in \mathbb{R}^d$. Let u and v be vertices of P such that $a^\mathsf{T} u < a^\mathsf{T} v$. Then there is a vertex w of P such that uw is an edge and $a^\mathsf{T} u < a^\mathsf{T} w$.*

Another way of formulating this is that if we consider the linear objective function $a^\mathsf{T} x$ on a polytope P, then from any vertex we can walk on the skeleton to a vertex that maximizes the objective function so that the value of the objective function increases at every step. This important fact is the basis for the *Simplex method*.

For our purposes, however, the following corollaries of Proposition 1.3.5 will be important:

Corollary 1.3.6 *The skeleton of any polytope is a connected graph.*

Corollary 1.3.7 *Let G be the skeleton of a d-polytope, and let H be an (open or closed) halfspace containing an interior point of the polytope. Then the subgraph of G_P induced by those vertices of P that are contained in this halfspace is connected.*

From Corollary 1.3.7, it is not hard to derive

Theorem 1.3.8 *The skeleton of a d-dimensional polytope is d-connected.*

1.3.3 Polar, blocker and antiblocker

Let P be a convex polytope containing the origin as an interior point. Then the *polar* of P is defined as

$$P^* = \{x \in \mathbb{R}^d : \; x^\mathsf{T} y \le 1 \forall y \in P\}$$

Proposition 1.3.9 *(a) The polar of a polytope is a polytope. For every polytope P we have $(P^*)^* = P$.*

(b) Let $v_0, \dots, v_m$ be the vertices of a k-dimensional face F of P. Then

$$F^\perp = \{x \in P^* : \ v_0^\mathsf{T} x = 1, \dots, v_m^\mathsf{T} x = 1\}$$

defines a $d - k - 1$-dimensional face of P^*. Furthermore, $(F^\perp)^\perp = F$.

In particular, every vertex v of P corresponds to a facet $v^\perp$ of P^* and vice versa. The vector v is a normal vector of the facet $v^\perp$.

There are two constructions similar to polarity that concern polyhedra that do not contain the origin in their interior; rather, they are contained in the nonnegative orthant.

A polyhedron P in $\mathbb{R}^d$ is called *ascending*, if $P \subseteq \mathbb{R}^d_+$ and whenever $x \in ¶$, $y \in \mathbb{R}^d$ and $y \geq x$ then $y \in P$.

The *blocker* of an ascending polyhedron is defined by

$$P^{\text{bl}} = \{x \in \mathbb{R}^d_+ : \ x^\mathsf{T} y \leq 1 \forall y \in P\}.$$

Proposition 1.3.10 *The blocker of an ascending polyhedron is an ascending polyhedron. For every ascending polyhedron P we have $(P^{\text{bl}})^{\text{bl}} = P$.*

The correspondence between faces of P and P^{bl} is a bit more complicated than for polarity, and we describe the relationship between vertices and facets only. Every vertex v of P gives rise to a facet $v\perp$, which corresponds to the halfspace $v^\mathsf{T} x \geq 1$. This construction gives all the facets of P^{bl}, except possibly those corresponding to the nonnegativity constraints $x_i \geq 0$, which may or may not define facets.

A d-polytope P is called a *corner polytope*, if $P \subseteq \mathbb{R}^d_+$ and whenever $x \in ¶$, $y \in \mathbb{R}^d$ and $0 \leq y \leq x$ then $y \in P$.

The *antiblocker* of a corner polytope is defined by

$$P^{\text{abl}} = \{x \in \mathbb{R}^d_+ : \ x^\mathsf{T} y \leq 1 \forall y \in P\}.$$

Proposition 1.3.11 *The antiblocker of a corner polytope is a corner polytope. For every corner polytope P we have $(P^{\text{abl}})^{\text{abl}} = P$.*

The correspondence between faces of P and P^{abl} is more complicated than for the blocking polyhedra. The nonnegativity constraints $x_i \geq 0$ always define facets, and they don't correspond to vertices in the antiblocker. All other facets of P correspond to vertices of P^{abl}. Not every vertex of P defines a facet in P^{abl}. The origin is a trivial exceptional vertex, but there may be further exceptional vertices. We call a vertex v *dominated*, if there is another vertex w such that $v \leq w$. Now a vertex of P defines a facet of P^* if and only if it is not dominated.

1.4 Semidefinite optimization

Linear programming has been one of the most fundamental and successful tools in optimization and discrete mathematics. Its applications include exact and approximation algorithms, as well as structural results and estimates. The key point is that linear programs are very efficiently solvable, and have a powerful duality theory.

Linear programs are special cases of convex programs; *semidefinite programs* are more general but still convex programs, to which many of the useful properties of linear programs extend. Recently, semidefinite programming arose as a generalization of linear programming with substantial novel applications. Again, it can be used both in proofs and in the design of exact and approximation algorithms. It turns out that various combinatorial optimization problems have semidefinite (rather than linear) relaxations which are still efficiently computable, but approximate the optimum much better. This fact has lead to a real breakthrough in approximation algorithms.

Semidefinite programs arise in a variety of ways: as certain geometric extremal problems, as relaxations (stronger than linear relaxations) of combinatorial optimization problems, in optimizing eigenvalue bounds in graph theory, as stability problems in engineering, etc.

For more comprehensive studies of issues concerning semidefinite optimization, see [189, 124].

1.4.1 Semidefinite programs

A semidefinite program is an optimization problem of the following form:

$$\begin{aligned} \text{minimize} \quad & c^{\mathsf{T}} x \\ \text{subject to} \quad & x_1 A_1 + \ldots x_n A_n - B \succeq 0 \end{aligned} \tag{1.17}$$

Here $A_1, \ldots, A_n, B$ are given symmetric $m \times m$ matrices, and $c \in \mathbb{R}^n$ is a given vector. We can think of $X = x_1 A_1 + \ldots x_n A_n - B$ as a matrix whose entries are linear functions of the variables.

As usual, any choice of the values x_i that satisfies the given constraint is called a *feasible solution.* A solution is *strictly feasible*, if the matrix X is positive definite. We denote by v_{primal} the supremum of the objective function.

The special case when $A_1, \ldots, A_n, B$ are diagonal matrices is just a "generic" linear program, and it is very fruitful to think of semidefinite programs as generalizations of linear programs. But there are important technical differences. The following example shows that, unlike in the case of linear programs, the supremum may be finite but not a maximum, i.e., not attained by any feasible solution.

Example 1.4.1 Consider the semidefinite program

$$\begin{aligned} \text{maximize} \quad & -x_1 \\ \text{subject to} \quad & \begin{pmatrix} x_1 & 1 & 0 \\ 1 & x_2 & 0 \\ 0 & 0 & x_1 \end{pmatrix} \succeq 0 \end{aligned}$$

The semidefiniteness condition boils down to the inequalities $x_1, x_2 \geq 0$ and $x_1 x_2 \geq 1$, so the possible values of the objective function are all negative real numbers. Thus $v_{\text{primal}} = 0$, but the supremum is not assumed.

As in the theory of linear programs, there are a large number of equivalent formulations of a semidefinite program. Of course, we could consider minimization instead of maximization. We could stipulate that the x_i are nonnegative, or more generally, we could allow additional linear constraints on the variables x_i (inequalities and/or equations). These could be incorporated into the form above by extending the A_i and B with new diagonal entries.

We could introduce the entries of A as variables, in which case the fact that they are linear functions of the original variables translates into linear relations between them. Straightforward linear algebra transforms (1.17) into an optimization problem of the form

$$\begin{array}{rl} \text{maximize} & C \cdot X \\ \text{subject to} & X \succeq 0 \\ & D_1 \cdot X = d_1 \\ & \vdots \\ & D_k \cdot X = d_k, \end{array} \tag{1.18}$$

where $C, D_1, \ldots, D_k$ are symmetric $m \times m$ matrices and $d_1, \ldots, d_k \in \mathbb{R}$. Note that $C \cdot X$ is the general form of a linear combination of entries of X, and so $D_i \cdot X = d_i$ is the general form of a linear equation in the entries of X.

It is easy to see that we would not get any substantially more general problem if we allowed linear inequalities in the entries of X in addition to the equations.

1.4.2 Fundamental properties of semidefinite programs

We begin with the semidefinite version of the Farkas Lemma:

Lemma 1.4.2 [Homogeneous version] *Let $A_1, \ldots, A_n$ be symmetric $m \times m$ matrices. The system*

$$x_1 A_1 + \cdots + x_n A_n \succ 0$$

has no solution in $x_1, \ldots, x_n$ if and only if there exists a symmetric matrix $Y \neq 0$ such that

$$\begin{array}{rcl} A_1 \cdot Y & = & 0 \\ A_2 \cdot Y & = & 0 \\ & \vdots & \\ A_n \cdot Y & = & 0 \\ Y & \succeq & 0 \,. \end{array}$$

There is an inhomogeneous version of this lemma.

Lemma 1.4.3 [Inhomogeneous version] *Let $A_1, \ldots, A_n, B$ be symmetric $m \times m$ matrices. The system*

$$x_1 A_1 + \ldots x_n A_n - B \succ 0$$

has no solution in $x_1, \ldots, x_n$ if and only if there exists a symmetric matrix $Y \neq 0$ such that

$$\begin{array}{rcl} A_1 \cdot Y & = & 0 \\ A_2 \cdot Y & = & 0 \\ & \vdots & \\ A_n \cdot Y & = & 0 \\ B \cdot Y & \geq & 0 \\ Y & \succeq & 0 \,. \end{array}$$

Given a semidefinite program (1.17), one can formulate the *dual program*:

$$\begin{aligned} \text{maximize} \quad & B \cdot Y \\ \text{subject to} \quad & A_1 \cdot Y = c_1 \\ & A_2 \cdot Y = c_2 \\ & \vdots \\ & A_n \cdot Y = c_m \\ & Y \succeq 0. \end{aligned} \tag{1.19}$$

Note that this too is a semidefinite program in the general sense. We denote by v_{dual} the infimum of the objective function.

With this notion of duality, the Duality Theorem holds in the following sense (see e.g. [187, 184, 185]):

Theorem 1.4.4 *Assume that both the primal and the dual semidefinite programs have feasible solutions. Then $v_{\text{primal}} \leq v_{\text{dual}}$. If, in addition, the primal program (say) has a strictly feasible solution, then the dual optimum is attained and $v_{\text{primal}} = v_{\text{dual}}$. In particular, if both programs have strictly feasible solutions, then the supremum resp. infimum of the objective functions are attained.*

The following *complementary slackness conditions* also follow from this argument.

Proposition 1.4.5 *Let x be a feasible solution of the primal program and Y, a feasible solution of the dual program. Then $v_{\text{primal}} = v_{\text{dual}}$ and both x and Y are optimal solutions if and only if $Y(\sum_i x_i A_i - B) = 0$.*

The following example shows that the somewhat awkward conditions about the strictly feasible solvability of the primal and dual programs cannot be omitted (see [149] for a detailed discussion of conditions for exact duality).

Example 1.4.6 Consider the semidefinite program

$$\begin{aligned} \text{minimize} \quad & x_1 \\ \text{subject to} \quad & \begin{pmatrix} 0 & x_1 & 0 \\ x_1 & x_2 & 0 \\ 0 & 0 & x_1+1 \end{pmatrix} \succeq 0 \end{aligned}$$

The feasible solutions are $x_1 = 0$, $x_2 \geq 0$. Hence v_{primal} is assumed and is equal to 0. The dual program is

$$\begin{aligned} \text{maximize} \quad & -Y_{33} \\ \text{subject to} \quad & Y_{12} + Y_{21} + Y_{33} = 1 \\ & Y_{22} = 0 \\ & Y \succeq 0 \,. \end{aligned}$$

The feasible solutions are all matrices of the form

$$\begin{pmatrix} a & 0 & b \\ 0 & 0 & 0 \\ b & 0 & 1 \end{pmatrix}$$

where $a \geq b^2$. Hence $v_{\text{dual}} = -1$.

1.4.3 Algorithms for semidefinite programs

There are two essentially different algorithms known that solve semidefinite programs in polynomial time: the *ellipsoid method* and *interior point/barrier methods*. Both of these have many variants, and the exact technical descriptions are quite complicated; so we restrict ourselves to describing the general principles underlying these algorithms, and to some comments on their usefulness. We ignore numerical problems, arising from the fact that the optimum solutions may be irrational and the feasible regions may be very small; we refer to [148, 149] for discussions of these problems.

The first polynomial time algorithm to solve semidefinite optimization problems in polynomial time was the ellipsoid method. Let K be a convex body (closed, compact, convex, full-dimensional set) in $\mathbb{R}^N$. We set $S(K,t) = \{x \in \mathbb{R}^N : d(x,K) \leq t\}$, where d denotes euclidean distance. Thus $S(0,t)$ is the ball with radius t about 0.

A *(weak) separation oracle* for a convex body $K \subseteq \mathbb{R}^N$ is an oracle whose input is a rational vector $x \in \mathbb{R}^N$ and a rational $\varepsilon > 0$; the oracle either asserts that $x \in S(K,\varepsilon)$ or returns an "almost separating hyperplane" in the form of a vector $0 \neq y \in \mathbb{R}^N$ such that $y^\mathsf{T} x > y^\mathsf{T} z - \varepsilon|y|$ for all $z \in K$.

If we have a weak separation oracle for a convex body (in practice, any subroutine the realizes this oracle) then we can use the ellipsoid method to optimize any linear objective function over K [75]:

Theorem 1.4.7 *Let K be a convex body in $\mathbb{R}^n$ and assume that we know two real numbers $R > r > 0$ such that $S(0,r) \subseteq K \subseteq S(0,R)$. Assume further that we have a weak separation oracle for K. Let a (rational) vector $c \in \mathbb{R}^n$ and an error bound $0 < \varepsilon < 1$ be also given. Then we can compute a (rational) vector $x \in \mathbb{R}^n$ such that $x \in K$ and $c^\mathsf{T} x \geq c^T z - \varepsilon$ for every $y \in K$. The number of calls on the oracle and the number of arithmetic operations in the algorithm are polynomial in* $\log(R/r) + \log(1/\varepsilon) + n$.

This method can be applied to solve semidefinite programs in polynomial time, modulo some technical conditions. (Note that some complications arise already from the fact that the optimum value is not necessarily a rational number, even if all parameters are rational. A further warning is example 1.4.6.)

Assume that we are given a semidefinite program (1.17) with rational coefficients and a rational error bound $\varepsilon > 0$. Also assume that we know a rational, strictly feasible solution $\tilde{x}$, and a bound $R > 0$ for the coordinates of an optimal solution. Then the set K of feasible solutions is a closed, convex, bounded, full-dimensional set in $\mathbb{R}^n$. It is easy to compute a small ball around x_0 that is contained in K.

The key step is to design a separation oracle for K. Given a vector x, we need only check whether $x \in K$ and if not, find a separating hyperplane. Ignoring numerical problems, we can use Gaussian elimination to check whether the matrix $Y = \sum_i x_i A_i - B$ is positive semidefinite. If it is, then $x \in K$. If not, the algorithm also returns a vector $v \in \mathbb{R}^m$ such that $v^\mathsf{T} Y v < 0$. Then $\sum_i x_i v^\mathsf{T} A_i v = v^\mathsf{T} B v$ is a separating hyperplane. (Because of numerical problems, the error bound in the definition of the weak separation oracle is needed.)

Thus using the ellipsoid method we can compute, in time polynomial in $\log(1/\varepsilon)$ and in the number of digits in the coefficients and in x_0, a feasible solution x such that the value of the objective function is at most $v_{\text{primal}} + \varepsilon$.

Unfortunately, the above argument gives an algorithm which is polynomial, but hopelessly slow, and practically useless. Still, the flexibility of the ellipsoid method makes it an inevitable tool in proving the *existence* (and not much more) of a polynomial time algorithm for many optimization problems.

Semidefinite programs can be solved in polynomial time and also *practically efficiently* by interior point methods [144, 2, 3]. The key to this method is the following property of the determinant of positive semidefinite matrices.

Lemma 1.4.8 *The function F defined by*

$$F(Y) = -\log\det\,(Y)$$

is convex and analytic in the interior of the semidefinite cone $\mathcal{P}_n$, and tends to ∞ at the boundary.

The algorithm can be described very informally as follows. The feasible domain of our semidefinite optimization problem is of the form $K = \mathcal{P}_n \cap A$, where A is an affine subspace of symmetric matrices. We want to minimize a linear function $C \cdot X$ over $X \in K$. The good news is that K is convex. The bad news is that the minimum will be attained on the boundary of K, and this boundary can have a very complicated structure; it is neither smooth nor polyhedral. Therefore, neither gradient-type methods nor the methods of linear programming can be used to minimize $C \cdot X$.

The main idea of barrier methods is that instead of minimizing $C^{\mathsf{T}}X$, we minimize the function $F_C(X) = F(X) + \lambda C^{\mathsf{T}}X$ for some $\lambda > 0$. Since F_λ tends to infinity on the boundary of K, the minimum will be attained in the interior. Since F_λ is convex and analytic in the interior, the minimum can be very efficiently computed by a variety of numerical methods (conjugate gradient etc.)

Of course, the point we obtain this way is not what we want, but if λ is large it will be close. If we don't like it, we can increase λ and use the minimizing point for the old F_λ as the starting point for a new gradient type algorithm. (In practice, we can increase λ after each iteration of this gradient algorithm.)

One can show that (under some technical assumptions about the feasible domain) this algorithm gives an approximation of the optimum with relative error ε in time polynomial in $\log(1/\varepsilon)$ and the size of the presentation of the program. The proof of this depends on a further rather technical property of the determinant, called "self-concordance". We don't go into the details, but refer to the articles [3, 184, 185] and the book [143].

1.4.4 Small dimension representations and rank minimization

If we consider a semidefinite relaxation of a discrete optimization problem (say, a 0-1 linear program), then typically the original solutions correspond to semidefinite matrices of rank 1. In linear programming, there are special but useful conditions that guarantee that the solutions of the relaxed linear problem are also solutions of the original integer problem (for example, perfectness, or total unimodularity). Can we find combinatorial conditions that guarantee that the semidefinite relaxation has a solution of rank 1? This question can be interesting for special combinatorial semidefinite relaxations.

If we find a solution that has, instead of rank 1, some other small rank, (i.e., a vector solution in low dimension), then this may decrease the error of the rounding methods, used to extract approximate solutions to the original problems. Thus the version of our question with "low rank" instead of "rank 1" also seems very interesting. One result in this direction is the following (discovered in many versions [17, 69, 146, 113]; see also [46], section 31.5, and [18]):

Theorem 1.4.9 *The semidefinite system*

$$
\begin{aligned}
&X \succeq 0\\
&D_1 \cdot X = d_1\\
&\vdots\\
&D_k \cdot X = d_k,
\end{aligned}
$$

has a solution of rank at most $\lceil\sqrt{2k}\rceil$.

Also from a geometric point of view, it is natural to consider unit distance (orthogonal, etc.) representations in a fixed small dimension. Without control over the rank of the solutions of semidefinite programs, this additional condition makes the use of semidefinite optimization methods very limited. On the other hand, several of these geometric representations of graphs are connected to interesting graph-theoretic properties, and some of them are related to semidefinite optimization. This connection is largely unexplored.

A final remark: many problems in graph theory, matroid theory, electrical engineering, static etc. can be formulated as *maximizing* the rank of a matrix subject to linear constraints (see [150, 121]). Such problems can be solved by an obvious randomized polynomial time algorithm, by substituting random numbers for the variables. Unlike in the case of the randomized algorithms described above for the Max Cut and other problems, it is not known whether these rank maximization problems can be solved in deterministic polynomial time.

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