Some Applications of Laplace Eigenvalues of Graphs*

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Abstract

In the last decade important relations between Laplace eigenvalues and eigenvectors of graphs and several other graph parameters were discovered. In these notes we present some of these results and discuss their consequences. Attention is given to the partition and the isoperimetric properties of graphs, the max-cut problem and its relation to semidefinite programming, rapid mixing of Markov chains, and to extensions of the results to infinite graphs.

1 Introduction

Applications of eigenvalue methods in combinatorics, graph theory and in combinatorial optimization have already a long history. For example, eigenvalue bounds on the chromatic number were formulated by Wilf [Wi] and Hoffman [Ho] already at the end of the sixties. Historically, the next applications related to combinatorial optimization, due to Fiedler [Fi1] and Donath and Hoffman [D-H] in 1973, concerned the area of graph partition. A very important use of eigenvalues is the Lovász' notion of the theta-function from 1979 [Lo]. Using it, he solved the long standing Shannon capacity problem for the 5-cycle. The theta-function provides the only known way to compute the chromatic number of perfect graphs in polynomial time.

The next important result was the use of eigenvalues in the construction of superconcentrators and expanders by Alon and Milman [A-M] in 1985. Their work motivated the study of eigenvalues of random regular graphs. Eigenvalues of random 01-matrices were studied already earlier by F. Juhász, who also analyzed the behavior of the theta-function on random graphs, and introduced eigenvalues in clustering [Ju]. Isoperimetric properties of graphs and their eigenvalues play a crucial role in the design of several randomized algorithms. These applications are based on the so-called rapidly mixing Markov chains. The most important discoveries in this area include random polynomial time algorithms for approximating the

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volume of a convex body (cf., e.g., [D-F-K, L-S1, L-S2]), polynomial time algorithms for approximate counting (e.g., approximating the permanent or counting the number of perfect matchings, see [Sin] for additional information), etc. Isoperimetric properties and related expansion properties of graphs are the basis for various other applications, ranging from the fast convergence of Markov chains, efficient approximation algorithms, randomized or derandomized algorithms, complexity lower bounds, and building efficient communication networks and networks for parallel computation.

There is an increasing interest in the application of eigenvalues in combinatorial optimization problems. To mention only some of them, Burkard, Finke, Rendl, and Wolkowicz [F-B-R, R-W] used the eigenvalue approach in the study of the quadratic assignment problem and general graph partition problems, Delorme and Poljak [D-P1, D-P2] in the max-cut problem, and Juvan and Mohar [J-M1, J-M2] in the labeling problems. Spectral partitioning which is based on eigenvectors of Laplace eigenvalues of graphs has proved to be one of the most successful heuristic approaches in the design of partition algorithms [B-S, H-L, H-M-P-R], in parallel computation [S-T, Sim, Wil], in solving sparse linear systems [P-S-W], clustering [H-K, C-S-Z] and in ranking [J-M2, H-M-P-R]. Similar kind of applications is based on the properties of the Perron-Frobenius eigenvector of a nonnegative matrix. This technique is suitable for the ranking problems. We refer to [M-P2] for additional applications.

There are several ways of using eigenvalues in the combinatorial optimization. The first possibility consists in formulating concrete bounds which involve eigenvalues of some related matrices. Examples of such bounds are given by the bounds on the separation properties in Section 3. Another way is to use the eigenvalues as a tool of transformation of combinatorial optimization problems to continuous optimization problems. Examples of this kind are provided by the bisection problem, max-cut problem, generalized partition problem, and the theta-function. The common point of these applications is the possibility of the change to a "continuous optimization", in particular to semidefinite programming. For example, in some cases there is a possibility of introducing a parameter $u \in \mathbf{R}^n$ and optimizing when u is restricted to be an element of a convex set $K \subseteq \mathbf{R}^n$. This way we get improved bounds or methods for the problems in question. A classical example is the Lovász' theta-function [Lo, G-L-S, Kn]. Its use gives rise to polynomial time algorithms for determining the stability number, or the chromatic number of perfect graphs. Similar approach appears in relation to the following problems: bipartition width, graph partition, and the max-cut problem (cf. Section 3), the bandwidth [J-M1, J-M2, H-M-P-R], etc. The max-cut problem and its relation to semidefinite programming is discussed in more details in Section 4.

In these notes we first discuss some results on Laplace matrices and Laplace eigenvalues of weighted graphs in the general framework. After introducing the Laplace matrix of a graph and presenting its basic properties in Section 2, relations between Laplace eigenvalues and separation properties of graphs are considered in Section 3. Section 4 discusses semidefinite programming and its relations to graph partitions. Random walks and associated matrices are treated in Section 5. The paper concludes by a brief introduction to Laplacians of infinite graphs in Section 6.

There are several existing books and survey papers concerning graph eigenvalues, e.g., [Bi, C-D-S, C-D-G-T, Fi3, Go, Mo3, M-P2, M-W]. We do not intend to overlap our presentation with their contents except partially with [M-P2]. Therefore we restrict ourselves to

some problems which can be classified as applications of eigenvalue methods in the design of algorithms and in combinatorial optimization. In particular, we do not include discussion on expander graphs (whose constructions are accessible only via eigenvalue methods) and their applications, although they are quite important tool in the design of algorithms and are extensively used in several other areas of theoretical computer science. Instead, we refer to the book [Lu1] by Lubotzky and to the notes of Lubotzky in this collection [Lu2].

2 The Laplacian of a graph

2.1 Basic notation

Let G be an undirected finite graph. By $V = V(G)$ and $E = E(G)$ we denote its vertex and edge set, respectively. Throughout these notes, the number of vertices and the number of edges of G are denoted by n and m, respectively. We also consider *weighted graphs*, i.e., graphs together with a *weight function*

$$w : V(G) \times V(G) \to \mathbf{R}^+$$

which assigns a nonnegative real weight $w(u, v)$ to each pair u, v of vertices. It is required that w satisfies the following properties:

(i) $w(u, v) > 0$ if $uv \in E(G)$, and $w(u, v) = 0$ if $uv \notin E(G)$.

(ii) $w(u, v) = w(v, u)$.

If $e = uv$ is an edge of G, property (ii) allows us to write $w(e)$ instead of $w(u, v)$. The weight $w(u, v)$ will also be denoted by a_{uv} (or a_{vu}). Unweighted graphs can be viewed as weighted graphs where $w(u, v)$ is equal to the number of edges between u and v.

In the unweighted case the degree d_u of the vertex $u \in V(G)$ is defined as the number of edges of G incident to u. In the weighted case we set

$$\mathrm{d}_u = \sum_{v \in V} w(u, v) = \sum_{v \in V} a_{uv} \, .$$

The maximum and the minimum vertex degree in G are denoted by $\Delta(G)$ and $\delta(G)$, respectively.

We will assume that the reader is familiar with basic notions of graph theory as found, e.g., in [B-M].

2.2 The Laplacian

Given a graph G, its (*weighted*) *adjacency matrix* $A(G) = [a_{uv}]$ is an $n \times n$ matrix with rows and columns indexed by $V(G)$ whose entries a_{uv} $(u, v \in V(G))$ are defined as above. Let $D(G) = \mathrm{diag}(\mathrm{d}_u; u \in V(G))$ be the diagonal matrix indexed by $V(G)$ and with vertex degrees on the diagonal. The difference

$$L(G) = D(G) - A(G) \tag{1}$$

is called the *Laplace matrix* of G (or the (*difference*) *Laplacian* of G). Historically, one of the first applications of Laplace matrices of graphs is in the proof of the well-known Matrix-Tree Theorem of Kirchhoff [Ki] (see also [Bi, Chapter 6]) which states that the number of

spanning trees in a graph G is equal to the cofactor of any element of the matrix $L(G)$. In particular, this gives a simple algebraic proof of Cayley formula [Ca] that there are n^{n-2} distinct labeled trees on n vertices.

Denote by Q an *oriented incidence matrix* of G which is defined as follows. Orient arbitrarily each edge of G. The matrix Q is an $n \times m$ matrix with rows and columns indexed by $V(G)$ and $E(G)$, respectively, and entries $(Q)_{ve}$ equal to $-\sqrt{w(e)}$ if v is the initial vertex of e, $\sqrt{w(e)}$ if v is the terminal vertex of e, and 0 otherwise. The last possibility also includes loops, irrespective of their weights.

PROPOSITION 2.1 *Let Q be an oriented incidence matrix with respect to some orientation of the edges of the graph G. Then*

$$L(G) = QQ^T . \tag{2}$$

PROOF. Given $u, v \in V(G)$ and $e \in E(G)$, it is easy to check that

$$(Q)_{ue}(Q^T)_{ev} = \begin{cases} -a_{uv}, & u \neq v \text{ and } u, v \text{ are the endvertices of } e \\ a_{uw}, & u = v \text{ and } e = uw, \text{ where } w \neq u \\ 0, & \text{otherwise.} \end{cases} \tag{3}$$

By summing up (3) over all edges of G, the proposition follows. □

Note that Proposition 2.1 also shows that the product QQ^T is independent of the chosen orientation of the edges of G.

Let $\mathbf{R}^V$ be the set of functions from V to $\mathbf{R}$,

$$\mathbf{R}^V = \{f : V \to \mathbf{R}\}.$$

If $f \in \mathbf{R}^V$ and $u \in V$, we shall use the notation f_u instead of the more customary $f(u)$ to denote the value of f at the vertex u. With the usual operations of the sum ($(f+g)_u = f_u + g_u$) and the multiplication by real numbers ($(\lambda f)_u = \lambda f_u$), $\mathbf{R}^V$ becomes a real vector space of dimension n endowed with the inner product

$$\langle f, g \rangle = \sum_{v \in V} f_v g_v.$$

The corresponding norm in $\mathbf{R}^V$ is

$$\|f\| = \langle f, f \rangle^{1/2} = \Big(\sum_{v \in V} f_v^2 \Big)^{1/2}.$$

The matrix $L = L(G)$ (and other matrices indexed by the vertices of G) acts on $\mathbf{R}^V$ as a linear operator. Its action is determined by the rule of matrix-vector multiplication, i.e., $g = Lf$ is the function defined by the formula

$$g_u = (Lf)_u = \sum_{v \in V} (L)_{uv} f_v \,, \qquad u \in V.$$

There is a natural quadratic form associated with $L = L(G)$:

PROPOSITION 2.2

$$\langle f, Lf\rangle = \sum_{uv\in E} a_{uv}(f_u - f_v)^2\,. \tag{4}$$

PROOF. Since $L = QQ^T$, the definition of Q implies

$$\langle f, Lf\rangle = \langle f, QQ^T f\rangle = \langle Q^T f, Q^T f\rangle = \sum_{e\in E}(Q^T f)_e^2 = \sum_{uv\in E} a_{uv}(f_u - f_v)^2\,.$$

□

Let us remark that in the case of an unweighted graph G, expression (4) reduces to

$$\langle f, Lf\rangle = \sum_{uv\in E} (f_u - f_v)^2\,. \tag{5}$$

2.3 Laplacians of graphs and Laplace operators on manifolds

Let M be a (compact) Riemannian manifold. The *Laplacian* Δ on M is the second order differential operator acting on $\mathcal{C}^\infty(M)$,

$$\Delta(\varphi) = -\mathrm{div}(\mathrm{grad}(\varphi)).$$

Let G be the graph of the triangulation of M. When looking for solutions of the Laplace equation

$$\Delta(\varphi) = \lambda\varphi \qquad (\varphi \in \mathcal{C}^\infty(M))$$

we may try to discretize the problem by looking on the restriction $f \in \mathbf{R}^V$ of φ to the vertex set V of G. For $uv \in E(G)$, define its weight as $a_{uv} = 1/(\rho(u,v))^2$ where $\rho(u,v)$ is the length of the edge uv in M. Let Q be the corresponding oriented incidence matrix of G. Then

$$(Q^T f)_{uv} = \frac{f_u - f_v}{\rho(u,v)}$$

is an approximation for the gradient of φ at the edge uv. Similarly, the corresponding Laplace matrix of G captures the properties of the Laplacian Δ on M: If the triangulation is "sufficiently fine", then the restriction of $\Delta\varphi$ to V and $L(G)f$ are close to each other.

There is another relationship between graphs and Riemannian manifolds that carries over to their Laplacians. We will briefly describe this relationship only in case of dimension 2 although it has obvious analogues for higher dimensions, too.

Let S be a surface of constant curvature -1 with three congruent boundary components such that S is homeomorphic to the "pair of pants" surface (the disk with two holes). If G is an arbitrary cubic graph, then we define a Riemannian surface $S(G)$ by taking a copy S_v of S for each vertex of G, and identifying the boundary circles of S_v in pairs with boundary circles in copies S_u of adjacent vertices u. This construction gives a surface of constant curvature -1 whose genus is equal to the cyclomatic number $g = |E(G)| - |V(G)| + 1$ of the graph G.

There is a close relationship between the Laplacian on $S(G)$ and the properties of the Laplace matrix of G. Moreover, some geometric properties of $S(G)$ are closely related to combinatorial properties of the graph. This relation gives an important bilateral link

between spectral geometry of Riemannian manifolds and graph theory. It makes possible to use results about graphs in the study of Laplacians on manifolds and, conversely, gives a possibility of transfering results about Laplacians on manifolds to graphs. Each of these directions has proved to be useful in research. We refer to the book by Buser [Bu] and to the paper [Br] for more details.

2.4 Laplace eigenvalues

By definition, $L(G)$ is a real symmetric matrix, and (4) (together with the nonnegativity of the edge-weights) implies that it is positive semidefinite. Therefore it has n nonnegative real eigenvalues $0 \leq \lambda_1 = \lambda_1(G) \leq \lambda_2 = \lambda_2(G) \leq \cdots \leq \lambda_n = \lambda_n(G)$ (repeated according to their multiplicities). These eigenvalues are called *Laplace eigenvalues* of the graph G. It is easy to see that 0 is always an eigenvalue of $L(G)$ and that $\mathbf{1} = (1, 1, \ldots, 1)^T$ is the corresponding eigenvector. More precisely, we have the following description of the multiplicity of 0 as an eigenvalue of $L(G)$.

PROPOSITION 2.3 *The multiplicity of the value* 0 *as an eigenvalue of* $L(G)$ *is equal to the number of connected components of* G.

PROOF. Let H be a connected component of G. Denote by $f^H \in \mathbf{R}^V$ the characteristic function of $V(H)$, i.e., the 0-1 function whose value f^H_v is equal to 1 if and only if $v \in V(H)$. Obviously, $L(G)f^H = 0$. Since the characteristic functions of different connected components are linearly independent, the multiplicity of the eigenvalue 0 is at least the number of connected components of G.

Conversely, let $f \in \mathbf{R}^V$ be a function from the kernel of $L(G)$. Then $\langle f, Lf \rangle = 0$, and (4) implies that f is constant on each connected component of G. Therefore f is a linear combination of the characteristic functions of connected components of G. □

In particular, Proposition 2.3 implies that $\lambda_1(G) = 0$ is a simple eigenvalue of $L(G)$ if and only if the graph G is connected.

If M is a matrix with real eigenvalues, we use the notation $\lambda_i(M)$ to denote the i-th smallest eigenvalue of M (respecting the multiplicities). To denote the maximal eigenvalue of M we will occasionally use the symbol $\lambda_{\max}(M)$. Consistently with this notation we may also write $\lambda_{\min}(M)$ instead of $\lambda_1(M)$.

Let G be a k-regular (weighted) graph, i.e., $\mathrm{d}_v = k$ for each $v \in V(G)$. Then (1) implies that λ is an eigenvalue of $L(G)$ if and only if $k - \lambda$ is an eigenvalue of the weighted adjacency matrix $A(G)$. More precisely,

$$\lambda_i(L(G)) = k - \lambda_{n+1-i}(A(G)), \qquad i = 1, \ldots, n. \tag{6}$$

This result enables us to use known results about the eigenvalues of the adjacency matrix of a regular graph in the study of its Laplace eigenvalues. We refer to [C-D-S] and to [Go] for numerous results on the adjacency matrix eigenvalues of graphs. For example, the eigenvalues of the adjacency matrix of the complete graph K_n are $n-1$ and -1 (the latter with multiplicity $n-1$). Therefore

$$\lambda_1(K_n) = 0, \text{ and } \lambda_k(K_n) = n \text{ for } 2 \leq k \leq n.$$

Similarly, the Laplace eigenvalues of the n-cycle C_n are precisely the numbers

$$\nu_k = 2 - 2\cos\Big(\frac{2k\pi}{n}\Big), \qquad k = 1, \ldots, n.$$

If G is a simple and unweighted graph and $\overline{G}$ is its complement, then

$$L(G) + L(\overline{G}) = nI - J \tag{7}$$

where J is the matrix with all entries equal to 1. Let $f^1, f^2, \ldots, f^n$ be an orthogonal system of eigenvectors of $L(G)$ such that $f^1 = \mathbf{1}$ and $L(G)f^i = \lambda_i f^i$ for $i = 1, \ldots, n$. By (7) we get $L(\overline{G})f^1 = 0$ and for $2 \le i \le n$,

$$L(\overline{G})f^i = (n - \lambda_i)f^i.$$

This shows that $\lambda_1(\overline{G}) = 0$ and that for $2 \le i \le n$ we have

$$\lambda_i(\overline{G}) = n - \lambda_{n-i+2}(G).$$

In particular, if $G = K_{n,m}$, then $\overline{G} = K_m \cup K_n$. So, $\overline{G}$ has eigenvalues $0^{(2)}, m^{(m-1)}, n^{(n-1)}$ (with the numbers in the superscripts indicating multiplicities). Hence the Laplace eigenvalues of $K_{n,m}$ are $0^{(1)}, n^{(m-1)}, m^{(n-1)}$, and $n + m$.

Let us recall that the *Cartesian product* $G \,\square\, H$ of graphs G and H has vertex set $V(G \,\square\, H) = V(G) \times V(H)$ where (u_1, u_2) is adjacent to (v_1, v_2) if and only if $u_1 = v_1$ and $u_2v_2 \in E(H)$ or $u_2 = v_2$ and $u_1v_1 \in E(G)$. There is a simple description of Laplace eigenvalues of $G \,\square\, H$ in terms of Laplace eigenvalues of G and H.

PROPOSITION 2.4 *The Laplace eigenvalues of the Cartesian product $G \,\square\, H$ are precisely the numbers*

$$\lambda_i(G) + \lambda_j(H) \quad (1 \le i \le |V(G)|, 1 \le j \le |V(H)|)$$

where each number is obtained as many times as is its multiplicity as an eigenvalue of $L(G \,\square\, H)$.

The proof of Proposition 2.4 relies on the fact that the Laplace matrix of $G \,\square\, H$ is equal to $L(G \,\square\, H) = L(G) \otimes I_{V(H)} + I_{V(G)} \otimes L(H)$, where $\otimes$ denotes the Kronecker product of matrices. The details are left to the reader.

Proposition 2.4 holds also for weighted graphs G and H if the weights of edges in $G \,\square\, H$ are determined by

$$w((u_1, u_2), (v_1, v_2)) = \begin{cases} w(u_1, v_1), & \text{if } u_2 = v_2 \\ w(u_2, v_2), & \text{if } u_1 = v_1 \\ 0, & \text{otherwise.} \end{cases}$$

As a consequence of Proposition 2.4 we obtain

$$\lambda_2(G \,\square\, H) = \min\{\lambda_2(G), \lambda_2(H)\}, \tag{8}$$

and

$$\lambda_{\max}(G \,\square\, H) = \lambda_{\max}(G) + \lambda_{\max}(H)\,. \tag{9}$$

Proposition 2.4 can be used to determine the Laplace spectrum of several well-known families of graphs.

EXAMPLE 2.5 The *d-dimensional hypercube* Q_d is the graph isomorphic to the Cartesian product of d copies of K_2. Since the Laplace eigenvalues of K_2 are 0 and 2, Proposition 2.4 asserts that the Laplace spectrum of Q_d consists of the numbers $2k$, $k = 0, 1, \ldots, d$. The multiplicity of $2k$ in the spectrum of Q_d is equal to $\binom{d}{k}$.

2.5 Bounding the Laplace eigenvalues

There are various useful min-max formulae for the expression of eigenvalues of a symmetric matrix. If M is a real symmetric matrix indexed by V, then

$$\begin{aligned} \lambda_1(M) &= \min\left\{\frac{\langle Mf, f\rangle}{\langle f, f\rangle} \mid 0 \neq f \in \mathbf{R}^V\right\} \\ &= \min\left\{\langle Mf, f\rangle \mid f \in \mathbf{R}^V,\, \|f\| = 1\right\} \end{aligned} \tag{10}$$

and similarly

$$\lambda_{\max}(M) = \max\left\{\langle Mf, f\rangle \mid f \in \mathbf{R}^V,\, \|f\| = 1\right\}. \tag{11}$$

The Rayleigh's characterization (10) has a generalization, the min-max characterization of the kth smallest eigenvalue $\lambda_k(M)$, known also as the Courant-Fisher's formula:

$$\lambda_k(M) = \min_U \max_f \left\{\langle Mf, f\rangle \mid \|f\| = 1,\ f \in U\right\} \tag{12}$$

where the minimum is taken over all k-dimensional subspaces U of $\mathbf{R}^V$. Another way of expressing (12) is

$$\lambda_k(M) = \min\left\{\langle Mf, f\rangle \mid \|f\| = 1, f \perp f_i, 1 \leq i < k\right\} \tag{13}$$

where $f_1, \ldots, f_{k-1}$ are pairwise orthogonal eigenvectors of $\lambda_1, \ldots, \lambda_{k-1}$, respectively.

Among the Laplace eigenvalues of G, the most important are the extreme nontrivial eigenvalues: the second smallest eigenvalue $\lambda_2(G)$ and the largest eigenvalue $\lambda_{\max}(G)$. (Let us observe that the relation (7) shows that $\lambda_2(G) = n - \lambda_{\max}(\overline{G})$. So, it is not surprising at all that the importance of one of these eigenvalues implies the importance of the other.) For a (weighted) graph G with Laplace matrix $L = L(G)$, (13) reads

$$\lambda_2(G) = \min\left\{\langle Lf, f\rangle \mid \|f\| = 1,\ f \perp \mathbf{1}\right\} \tag{14}$$

since $\mathbf{1}$ is an eigenvector corresponding to $\lambda_1(G)$. Let us observe that f is orthogonal to $\mathbf{1}$ if and only if the sum of the values of f is 0, $\sum_{v\in V} f_v = 0$. Expression (14) can be used to get combinatorial upper bounds on $\lambda_2(G)$. For example:

LEMMA 2.6 *Let $s, t \in V(G)$ be nonadjacent vertices of a graph G. Then*

$$\lambda_2(G) \leq \frac{1}{2}(\mathrm{d}_s + \mathrm{d}_t).$$

PROOF. Let $f \in \mathbf{R}^V$ be defined by

$$f_v = \begin{cases} 1, & v = s \\ -1, & v = t \\ 0, & \text{otherwise.} \end{cases}$$

Since $f \perp \mathbf{1}$, (14) yields

$$\lambda_2(G) \leq \frac{\langle L(G)f, f\rangle}{\langle f, f\rangle} = \frac{\sum_{uv\in E} a_{uv}(f_u - f_v)^2}{\sum_{v\in V} f_v^2} = \frac{\mathrm{d}_s + \mathrm{d}_t}{2}\,.$$

□

The proof of Lemma 2.6 presents a basic technique to exploit expressions like (14). By inserting an appropriate function in the expression, the right-hand side gets a meaningful combinatorial interpretation, and this enables us to relate combinatorial properties in question with the Laplace eigenvalues. To overcome the orthogonality restriction on f, Fiedler [Fi2] transformed (14) to a more suitable expression which does not require f to be orthogonal to $\mathbf{1}$ in order to be applied.

Proposition 2.7

$$\lambda_2(G) = 2n \cdot \min\left\{ \frac{\sum\limits_{uv\in E} a_{uv}(f_u - f_v)^2}{\sum\limits_{u\in V}\sum\limits_{v\in V}(f_u - f_v)^2} \;\middle|\; f \neq c\mathbf{1} \text{ for } c \in \mathbf{R} \right\}. \tag{15}$$

Proof. Observe first that both the numerator and the denominator of the fraction in the minimum are invariant for the addition of a constant function. This observation together with (4) and (14) implies that it suffices to show that $2n\langle f, f\rangle = \sum_{u\in V}\sum_{v\in V}(f_u - f_v)^2$ whenever f is orthogonal to $\mathbf{1}$. So, assume that $f \perp \mathbf{1}$. Then

$$\begin{aligned}\sum_{u\in V}\sum_{v\in V}(f_u - f_v)^2 &= \sum_{u\in V}\sum_{v\in V} f_u^2 - 2\sum_{u\in V}\sum_{v\in V} f_u f_v + \sum_{u\in V}\sum_{v\in V} f_v^2 \\ &= 2n\langle f, f\rangle - 2\langle f, \mathbf{1}\rangle^2 = 2n\langle f, f\rangle\,.\end{aligned}$$

□

An almost identical proof yields a similar expression for $\lambda_{\max}(G)$:

$$\lambda_{\max}(G) = 2n \cdot \max\left\{ \frac{\sum\limits_{uv\in E} a_{uv}(f_u - f_v)^2}{\sum\limits_{u\in V}\sum\limits_{v\in V}(f_u - f_v)^2} \;\middle|\; f \neq c\mathbf{1} \text{ for } c \in \mathbf{R} \right\}. \tag{16}$$

Let us conclude this section by presenting bounds on $\lambda_2(G)$ and $\lambda_{\max}(G)$ in terms of maximum and minimum degrees of G.

Proposition 2.8

$$\lambda_2(G) \leq \frac{n}{n-1}\delta(G) \leq \frac{n}{n-1}\Delta(G) \leq \lambda_{\max}(G) \leq 2\Delta(G). \tag{17}$$

Proof. Choose a vertex $v \in V(G)$ and let $e^{(v)} \in \mathbf{R}^V$ be the function of the standard base corresponding to v, i.e., $e_v^{(v)} = 1$ and $e_u^{(v)} = 0$ for each $u \neq v$. By putting $e^{(v)}$ in (15), we get

$$\lambda_2(G) \leq 2n\frac{\mathrm{d}_v}{2(n-1)} = \frac{n}{n-1}\mathrm{d}_v\,.$$

Since v was chosen arbitrarily, the first inequality follows. The lower bound on $\lambda_{\max}(G)$ is proved analogously using (16).

It remains to show that $\lambda_{\max}(G) \leq 2\Delta(G)$. Since the matrix $\Delta(G)I_{V(G)} - L(G)$ is (elementwise) nonnegative, Perron-Frobenius theorem implies that its largest eigenvalue $\Delta(G)$ is greater than or equal to the absolute value of its smallest eigenvalue, i.e., $\Delta(G) \geq |\Delta(G) - \lambda_{\max}(G)|$. In particular, $\Delta(G) \geq \lambda_{\max}(G) - \Delta(G)$ as claimed. □

An alternative proof of the first part of Proposition 2.8 can be obtained by showing that the matrices $L(G) - \lambda_2(G)(I - \frac{1}{n}\mathbf{1}\,\mathbf{1}^T)$ and $\lambda_{\max}(G)(I - \frac{1}{n}\mathbf{1}\,\mathbf{1}^T) - L(G)$ are positive semidefinite and by considering their diagonal entries.

The application of the Perron-Frobenius theorem in the proof of the last inequality in Proposition 2.8 can be strengthened to show that for a connected graph G, $\lambda_{\max}(G) = 2\Delta(G)$ if and only if G is a bipartite $\Delta(G)$-regular graph. See, for example, [Go].

3 Partitions of graphs

3.1 Edge cuts and eigenvalues

For a subset $S \subseteq V(G)$, let $\bar{S} = V(G)\backslash S$ denote the complement of S in $V(G)$. Given sets of vertices $A, B \subseteq V(G)$, let $E(A, B)$ be the set of those edges of G that have one endvertex in A and the other in B. We also set

$$e(A, B) = \sum_{u \in A} \sum_{v \in B} w(u, v) = \sum_{e \in E(A,B)} w(e)$$

to be the sum of the weights of the edges in $E(A, B)$. Note that for an unweighted graph G, $e(S, \bar{S})$ counts the number of edges in the cut $E(S, \bar{S})$.

The partition problems discussed in this section are mainly concerned with finding an appropriate subset $S \subseteq V(G)$ such that the edge cut $E(S, \bar{S})$ satisfies some specific extremal property. In particular, we focus our attention to the following quantities: the weight of a maximum cut, the bipartition width, and the isoperimetric number. The computational complexity of these problems is such that there is no hope of finding an optimal solution to a moderately sized problem in a reasonable amount of time. (More precisely, they are NP-hard.) Therefore any nontrivial bounds are desirable and potentially very important.

Let us start by a lemma that relates the weight of an edge cut $E(S, \bar{S})$ to the eigenvalues $\lambda_2(G)$ and $\lambda_{\max}(G)$ of the Laplacian of the underlying graph. Although simple to prove, the lemma is a fundamental tool for obtaining bounds on various graph properties related to partitions.

LEMMA 3.1 *Let G be a (weighted) graph of order n and $S \subseteq V(G)$. Then*

$$\lambda_2(G)\frac{|S|(n - |S|)}{n} \leq e(S, \bar{S}) \leq \lambda_{\max}(G)\frac{|S|(n - |S|)}{n}\,.$$

PROOF. Let $f \in \mathbf{R}^V$ be the characteristic function of S, i.e., $f_v = 1$ if $v \in S$ and $f_v = 0$ otherwise. Then

$$\sum_{u \in V} \sum_{v \in V} (f_u - f_v)^2 = 2|S|(n - |S|)$$

and

$$\sum_{uv \in E} a_{uv}(f_u - f_v)^2 = e(S, \bar{S})\,.$$

If $S \neq \emptyset$ and $S \neq V(G)$, (15) implies

$$\lambda_2(G) \leq 2n \cdot \frac{e(S, \bar{S})}{2|S|(n - |S|)}\,.$$

After rearranging, this gives the lower bound. Obviously, the lower bound also holds for $S = \emptyset$ and $S = V(G)$. The upper bound is proved analogously using (16). □

It is an immediate, and also an important consequence of Lemma 3.1 that in a graph with all non-trivial Laplace eigenvalues being close together, i.e., when $\lambda_{\max} - \lambda_2$ is small, the weights of all edge cuts $E(S, \bar{S})$ corresponding to vertex sets S of the same cardinality are approximately the same. In particular, this property holds for the cardinalities of edge cuts in random graphs. Therefore it is not surprising that many algorithms dealing with edge cuts perform very well on randomly chosen graphs.

3.2 The bipartition width

Let G be a graph of order n. The *bipartition width* $\mathrm{bw}(G)$ of the graph G is defined as

$$\mathrm{bw}(G) = \min\{e(S, \bar{S}) \mid S \subseteq V(G), |S| = \lfloor n/2 \rfloor\}\,.$$

In the unweighted case, the bipartition width of the graph G is equal to the minimum number of edges whose deletion disconnects G into two parts of the same size (up to a vertex). It is known that even for unweighted simple graphs the problem of determining $\mathrm{bw}(G)$ is NP-hard (see, e.g., [G-J, p. 210]).

Let us remark that the "reversed" problem of determining

$$\overline{\mathrm{bw}}(G) = \max\{e(S, \bar{S}) \mid S \subseteq V(G), |S| = \lfloor n/2 \rfloor\}$$

is closely related to the original one. Namely, given a weighted graph G with weight function w, let $W = \max\{a_{uv} \mid u, v \in V(G)\}$. Define the "weighted complement" of G as the weighted graph $\bar{G}$ with $V(\bar{G}) = V(G)$ and the weight function $\bar{w}(u, v) = W - w(u, v)$. Then

$$\mathrm{bw}(G) + \overline{\mathrm{bw}}(\bar{G}) = W \cdot \left\lfloor \frac{n}{2} \right\rfloor \left\lceil \frac{n}{2} \right\rceil$$

which implies that the problems of determining bw and $\overline{\mathrm{bw}}$ are actually equivalent.

Since all the sets, over which the minimum in the definition of $\mathrm{bw}(G)$ is taken, have size $\lfloor n/2 \rfloor$, Lemma 3.1 gives the following lower bound on $\mathrm{bw}(G)$.

COROLLARY 3.2 *Let G be a weighted graph of order n. If n is even, then*

$$\mathrm{bw}(G) \geq \frac{n}{4} \cdot \lambda_2(G)\,. \tag{18}$$

If n is odd, then

$$\mathrm{bw}(G) \geq \frac{n^2 - 1}{4n} \cdot \lambda_2(G)\,. \tag{19}$$

The bounds of Corollary 3.2 can be further improved by introducing a correction function. A function $c \in \mathbf{R}^V$ is called a *correction function* if $c \perp \mathbf{1}$. The following bound was proved by Boppana [Bo].

PROPOSITION 3.3 *Let G be a weighted graph of even order n. Then*

$$\mathrm{bw}(G) \geq \frac{n}{4} \cdot \max_c \min_f \frac{\langle (L(G) + \mathrm{diag}(c))f, f\rangle}{\langle f, f\rangle} \tag{20}$$

where the maximum is taken over all correction functions $c \in \mathbf{R}^V$ and the minimum is taken over all nonzero functions $f \in \mathbf{R}^V$ with $f \perp \mathbf{1}$.

PROOF. Let $S \subseteq V(G)$ be a set of cardinality $\frac{n}{2}$ with $e(S, \bar{S}) = \mathrm{bw}(G)$ and let $g \in \mathbf{R}^V$ be its signed characteristic function, i.e., the function defined by $g_v = 1$ if $v \in S$ and $g_v = -1$ if $v \in \bar{S}$. Since $|S| = |\bar{S}|$, $g \perp \mathbf{1}$. Take an arbitrary correction function $c \in \mathbf{R}^V$. Since $c \perp \mathbf{1}$, we have

$$\langle \mathrm{diag}(c)g, g\rangle = \sum_{v \in V} c_v g_v^2 = \sum_{v \in V} c_v = 0\,. \tag{21}$$

Using (21) and applying (4) we get

$$\begin{aligned} \frac{\langle (L(G) + \mathrm{diag}(c))g, g\rangle}{\langle g, g\rangle} &= \frac{\langle L(G)g, g\rangle}{\langle g, g\rangle} = \frac{\sum_{uv \in E} a_{uv}(g_u - g_v)^2}{\sum_{v \in V} g_v^2} \\ &= \frac{4e(S, \bar{S})}{n} = \frac{4}{n} \cdot \mathrm{bw}(G). \end{aligned}$$

Since c was arbitrary, the bound follows. □

For computational purposes, it is convenient to express the bound of Proposition 3.3 as a maximization of the smallest eigenvalue of an appropriate symmetric matrix. This can be done as follows. Let $Q = (q_1, \ldots, q_{n-1})$ be an $n \times (n-1)$ matrix such that the columns q_i are pairwise orthogonal unit vectors with the property that $q_i \perp \mathbf{1}$ $(1 \leq i < n)$. It is easy to see that for every $x \in \mathbf{R}^{n-1}$ we have $\langle Qx, Qx\rangle = \langle x, x\rangle$ and $Qx \perp \mathbf{1}$. This implies:

COROLLARY 3.4 *We have*

$$\mathrm{bw}(G) \geq \frac{n}{4} \cdot \max_c \lambda_{\min}(Q^T(L(G) + \mathrm{diag}(c))Q)$$

where the maximum is taken over all correction functions $c \in \mathbf{R}^V$.

We shall see in Section 4 that the bound of Corollary 3.4 can be formulated as a semidefinite program, and can therefore be computed to an arbitrary precision in polynomial time using known polynomial time methods for solving such programs.

3.3 The max-cut problem

The *maximum cut* (or *max-cut*) *problem* is similar to the "reversed" bipartition width problem except that the restrictions on the sizes of the subsets over which the maximum is taken are omitted. More precisely, let $\mathrm{mc}(G)$ denote the maximum weight of an edge cut in G,

$$\mathrm{mc}(G) = \max\{e(S, \bar{S}) \mid \emptyset \neq S \subset V(G)\}.$$

As far as the computational complexity is concerned, the problem of determining $\mathrm{mc}(G)$ is NP-hard [Karp] (see also [G-J, p. 210]). Even more, it is known that there exists a constant $\varepsilon > 0$ such that there is no polynomial time $(1-\varepsilon)$-approximation algorithm for the max-cut problem unless $P = NP$ [P-Y, A-L-M-S-S]. On the other hand, we will see in Section 4 that it is possible to find a 0.878-approximation to $\mathrm{mc}(G)$ in polynomial time. Unlike the bipartition width problem, the "reversed" problem of max-cut, the *minimum cut problem*, which requires to determine

$$\min\{e(S, \bar{S}) \mid \emptyset \neq S \subset V(G)\},$$

is easy to solve in polynomial time using standard flow techniques.

Lemma 3.1 implies the following upper bound on $\mathrm{mc}(G)$ which was first observed by Mohar and Poljak [M-P1].

COROLLARY 3.5 *Let G be a weighted graph of order n. Then*

$$\mathrm{mc}(G) \leq \frac{n}{4} \cdot \lambda_{\max}(G). \tag{22}$$

Similarly to the bipartition width problem, the bound (22) can be further improved using correction functions. The following eigenvalue bound was introduced by Delorme and Poljak [D-P1].

PROPOSITION 3.6 *Let G be a weighted graph of order n. Then*

$$\mathrm{mc}(G) \leq \frac{n}{4} \cdot \min_{c} \lambda_{\max}(L(G) + \mathrm{diag}(c)) \tag{23}$$

where the minimum is taken over all correction functions $c \in \mathbf{R}^V$.

PROOF. The proof consists of similar steps as the proof of Proposition 3.3. Choose $S \subset V(G)$ such that $e(S, \bar{S}) = \mathrm{mc}(G)$ and let $g \in \mathbf{R}^V$ be the signed characteristic function of S, i.e., $g_v = 1$ if $v \in S$ and $g_v = -1$ if $v \in \bar{S}$. Take an arbitrary correction function $c \in \mathbf{R}^V$. As in the proof of Proposition 3.3, we have

$$\langle \mathrm{diag}(c)g, g\rangle = 0$$

and

$$\frac{\langle (L(G) + \mathrm{diag}(c))g, g\rangle}{\langle g, g\rangle} = \frac{4e(S, \bar{S})}{n} = \frac{4}{n} \cdot \mathrm{mc}(G).$$

Since

$$\frac{\langle (L(G) + \mathrm{diag}(c))g, g\rangle}{\langle g, g\rangle} \leq \lambda_{\max}(L(G) + \mathrm{diag}(c))$$

and c was chosen arbitrarily, the bound follows. □

The performance of (23) was investigated in [D-P2]. It will be further discussed in Section 4 where it will be formulated as a semidefinite program.

3.4 Edge-forwarding index

An important notion used in the theory of communication networks is the forwarding index of a graph. A relation between the forwarding index and the Laplace eigenvalues was observed by Solé [So].

Let G be a connected graph and suppose that for each (ordered) pair u, v of distinct vertices of G we have a path $R_{u,v}$ from u to v. The collection of paths

$$\mathcal{R} = \{R_{u,v} \mid u, v \in V(G), u \neq v\}$$

is called a *routing* in G. For each $e \in E(G)$, denote by $\xi(G, \mathcal{R}, e)$ the number of paths $R_{u,v}$ which contain the edge e. Let

$$\xi(G, \mathcal{R}) = \max\{\xi(G, \mathcal{R}, e) \mid e \in E(G)\}.$$

The minimum

$$\xi(G) = \min \xi(G, \mathcal{R})$$

taken over all routings $\mathcal{R}$ of G is called the *edge-forwarding index* of G. The edge-forwarding index is an important parameter in the study of communication networks (see, e.g., [C-C-R-S, H-M-S] or the notes of Heydemann [He] in this collection).

PROPOSITION 3.7 *Let G be unweighted connected graph of order n with the edge-forwarding index $\xi(G)$, and let $S \subseteq V(G)$. Then*

$$\xi(G) \geq \frac{2|S|(n - |S|)}{e(S, \bar{S})} \geq \frac{2n}{\lambda_{\max}(G)}\,.$$

PROOF. Let $\mathcal{R}$ be a routing. Each path in $\mathcal{R}$ joining a vertex of S with a vertex in $\bar{S}$ contains at least one edge in $E(S, \bar{S})$. Since there are $2|S|(n - |S|)$ such paths, this proves the first inequality. The second inequality follows by Lemma 3.1. □

3.5 Isoperimetric inequalities

Isoperimetric problems are related to questions in which one considers the ratio between the surface area and the volume of d-dimensional bodies or more general (Riemannian) manifolds. In graph theory, natural analogue to the volume is the number of vertices or the sum of vertex degrees in a subset S of vertices of the graph, while the counterpart for the measure of the surface area is the number $e(S, \bar{S})$ of the edges with one end in S and the other end outside the set S. Problems in which one considers ratios of the form $e(S, \bar{S})/|S|$ are therefore called isoperimetric problems for graphs. In other words, isoperimetric properties concern the sizes of the neighborhood of a set of vertices. The related term "expansion" usually means that the sizes of the neighborhood can be bounded from below by some function of the size of the subset. Such isoperimetric properties provide the foundation for many recent developments in applications of graph theory in theoretical computer science which are mentioned in the introduction.

The *isoperimetric number* $i(G)$ of a graph G of order $n \geq 2$ is defined as

$$i(G) = \min\left\{\frac{e(S, \bar{S})}{|S|} \;\middle|\; S \subset V(G), 0 < |S| \leq \frac{n}{2}\right\}.$$

Computationally the problem of determining $i(G)$ is NP-hard [Mo2]. Let us remark that a seemingly related quantity

$$\max\left\{\frac{e(S,\bar{S})}{|S|}\;\Big|\;S\subset V(G), 0<|S|\le\frac{n}{2}\right\}$$

is not very interesting since it is always equal to $\Delta(G)$.

A straightforward application of Lemma 3.1 yields the following eigenvalue lower bound on $i(G)$.

COROLLARY 3.8 *Let G be a weighted graph of order n. Then*

$$i(G)\ge\frac{\lambda_2(G)}{2}\,.$$

PROOF. Let $S\neq\emptyset$ be a set of vertices. By Lemma 3.1, we have

$$\frac{e(S,\bar{S})}{|S|}\ge\lambda_2(G)\frac{n-|S|}{n}\,.$$

If $|S|\le\frac{n}{2}$, then $(n-|S|)/n\ge 1/2$. This implies the bound on $i(G)$. □

It is difficult to obtain useful lower bounds on $i(G)$ by combinatorial means. On the other hand, Corollary 3.8, although easy to prove, gives a nontrivial lower bound on $i(G)$. Let us present an example where the bound of Corollary 3.8 is, in fact, tight.

EXAMPLE 3.9 Take the d-dimensional cube $Q_d=K_2\,\square\,Q_{d-1}$ and let $S=\{0\}\times Q_{d-1}$. Since $|S|=e(S,\bar{S})=2^{d-1}$, $i(Q_d)\le 1$. On the other hand, we know from Example 2.5 that $\lambda_2(Q_d)=2$. Using Corollary 3.8 we conclude that $i(Q_d)=1$.

The following quantity is sometimes easier to deal with than $i(G)$:

$$i^*(G)=\min\Big\{\frac{e(S,\bar{S})}{|S|\,|\bar{S}|}\cdot\frac{|V|}{2}\;\Big|\;\emptyset\neq S\subset V\Big\}.$$

Clearly, $i(G)/2\le i^*(G)\le i(G)$. It turns out that $i^*(G)$ satisfies a relation similar to (8):

$$i^*(G\,\square\,H)=\min\{i^*(G),i^*(H)\}.$$

A proof of this can be found in [H-T]; see also [C-T].

The above inequality implies

$$\frac{1}{2}\min\{i(G),i(H)\}\le i(G\,\square\,H)\le\min\{i(G),i(H)\}.$$

While the inequality on the right can be strict (see [Mo2]), it is not known whether the factor $\frac{1}{2}$ on the left is the best possible constant.

Corollary 3.8 may be used to get bounds on $i(G)$ since λ_2 is usually easier to compute (or to estimate) than $i(G)$. Sometimes, however, one can estimate $i(G)$, while a bound on λ_2 is desired. (Such examples appear, for instance, in the study of the rate of convergence of Markov chains; cf. Section 5.) In such a case, one would like to use converse inequality,

obtaining an upper bound on $i(G)$ in terms of $\lambda_2(G)$. Such inequalities are known as *Cheeger inequalities* since they are discrete analogues of their continuous counterpart [Che] (see also [Br, Bu, Cha]) arising in the study of Laplace operators on Riemannian manifolds.

The classical form of Cheeger's bound adapted to graphs reads as

$$i(G) \le \sqrt{2\Delta(G)\lambda_2(G)}\,. \tag{24}$$

In the sequel we shall present an improved eigenvalue upper bound of Cheeger's type from [Mo2].

THEOREM 3.10 *Let G be a weighted graph of order n, $G \neq K_n$, and let $\Delta = \Delta(G)$ and $\lambda_2 = \lambda_2(G)$. Then*

$$i(G) \le \sqrt{(2\Delta - \lambda_2)\lambda_2}\,.$$

PROOF. Since for a disconnected graph G we have $\lambda_2 = i(G) = 0$, we may assume that G is connected. Let f be an eigenfunction of $L(G)$ corresponding to λ_2. Set $W = \{v \in V(G) \mid f_v > 0\}$. After possible replacement of f by $-f$ we may assume that $|W| \le \frac{n}{2}$. Let $g \in \mathbf{R}^V$ be defined by $g_v = f_v$ if $v \in W$ and $g_v = 0$ otherwise. Then

$$\begin{aligned}
\lambda_2 \sum_{u\in W} f_u^2 &= \sum_{u\in W} (Lf)_u f_u = \sum_{u\in W} \Big(\mathrm{d}_u f_u - \sum_{v\in V} a_{uv} f_v\Big) f_u \\
&= \sum_{u\in W}\sum_{v\in V} a_{uv}(f_u - f_v) f_u \\
&= \sum_{u\in W}\sum_{v\in W} a_{uv}(f_u - f_v) f_u + \sum_{u\in W}\sum_{v\notin W} a_{uv}(f_u - f_v) f_u \\
&\ge \sum_{u\in W}\sum_{v\in W} a_{uv}(f_u - f_v) f_u + \sum_{u\in W}\sum_{v\notin W} a_{uv} f_u^2 \\
&= \sum_{uv\in E(W,W)} a_{uv}(g_u - g_v)^2 + \sum_{uv\in E(W,\bar{W})} a_{uv}(g_u - g_v)^2 \\
&= \sum_{uv\in E} a_{uv}(g_u - g_v)^2 = \langle Lg, g\rangle\,.
\end{aligned}$$

Since $\sum_{v\in W} f_v^2 = \sum_{v\in V} g_v^2 = \langle g, g\rangle$, we have

$$\lambda_2 \ge \frac{\langle Lg, g\rangle}{\langle g, g\rangle} =: K\,.$$

Then

$$\begin{aligned}
\sum_{uv\in E} a_{uv}(g_u + g_v)^2 &= 2\sum_{uv\in E} a_{uv}(g_u^2 + g_v^2) - \sum_{uv\in E} a_{uv}(g_u - g_v)^2 \\
&= 2\sum_{v\in V} \mathrm{d}_v g_v^2 - \langle Lg, g\rangle \le 2\Delta \sum_{v\in V} g_v^2 - \langle Lg, g\rangle \\
&= (2\Delta - K)\langle g, g\rangle.
\end{aligned}$$

This inequality together with the Cauchy-Schwartz inequality implies

$$\begin{aligned} K &= \frac{\sum_{uv\in E} a_{uv}(g_u-g_v)^2 \sum_{uv\in E} a_{uv}(g_u+g_v)^2}{\langle g,g\rangle \sum_{uv\in E} a_{uv}(g_u+g_v)^2} \\ &\geq \frac{\Big(\sum_{uv\in E} a_{uv}|g_u^2-g_v^2|\Big)^2}{(2\Delta-K)\langle g,g\rangle^2}\,. \end{aligned} \tag{25}$$

The quantity

$$M := \sum_{uv\in E} a_{uv}|g_u^2-g_v^2|$$

can be interpreted as a measure of optimality of the partitions of V determined by λ_2 and f. A lower bound on M in terms of the isoperimetric number can be obtained in a similar manner as in the setting of Riemannian manifolds. The following calculation is a discrete analogue of the integration per partes. Let $0 = t_0 < t_1 < \cdots < t_m$ be all distinct values of g_v ($v \in V$). For $k = 0, 1, \ldots, m$, let $V_k := \{v \in V \mid g_v \geq t_k\}$. Note that $|V_k| \leq |W| \leq \frac{n}{2}$ if $k > 0$. Then

$$\begin{aligned} M &= \sum_{uv\in E} a_{uv}|g_u^2-g_v^2| = \sum_{k=1}^{m} \sum_{\substack{uv\in E \\ g_v<g_u=t_k}} a_{uv}(g_u^2-g_v^2) \\ &= \sum_{k=1}^{m} \sum_{\substack{g_u=t_k \\ g_v=t_l, l<k}} a_{uv}(t_k^2 - t_{k-1}^2 + t_{k-1}^2 - \cdots - t_{l+1}^2 + t_{l+1}^2 - t_l^2) \\ &= \sum_{k=1}^{m} \sum_{u\in V_k} \sum_{v\notin V_k} a_{uv}(t_k^2 - t_{k-1}^2) \\ &= \sum_{k=1}^{m} e(V_k, \bar{V}_k)\cdot(t_k^2 - t_{k-1}^2) \\ &\geq i(G) \sum_{k=1}^{m} |V_k|(t_k^2 - t_{k-1}^2) = i(G) \sum_{k=1}^{m} t_k^2(|V_k| - |V_{k+1}|) \\ &= i(G) \sum_{v\in W} g_v^2\,. \end{aligned} \tag{26}$$

In the last line we used the fact that $|V_{m+1}| = 0$.

Combining (25) and (26), we get

$$K \geq \frac{i(G)^2}{2\Delta - K}\,. \tag{27}$$

Since $\lambda_2 \geq K$, (27) implies

$$\lambda_2 \geq \Delta - \sqrt{\Delta^2 - i(G)^2}\,. \tag{28}$$

Since $G \neq K_n$, Lemma 2.6 shows that $\lambda_2 \leq \Delta$. Rearranging (28), this inequality finally yields $i^2(G) \leq (2\Delta - \lambda_2)\lambda_2$. □

Let us note that the bound of Theorem 3.10 also holds for $G = K_n$ if $n \geq 3$.

Other forms of discrete Cheeger's inequalities have been proved by Alon [Alo], Mohar [Mo1], Sinclair and Jerrum [S-J], Diaconis and Stroock [D-St], Chung [Chu], and others. See also Section 6.

By using (14), inequality (24) can be expressed as follows:

$$\frac{i^2(G)}{2\Delta(G)} \leq \min\Big\{ \frac{\sum_{uv\in E} a_{uv}(f_u - f_v)^2}{\sum_{v\in V} f_v^2} \,\Big|\, f \in \mathbf{R}^V, f \perp \mathbf{1} \Big\}.$$

Recent results of [H-T] provide a generalization of the above inequality by replacing the right hand side by the pth powers of ℓ_p-norms (and more generally to Orlicz norms), and replacing the constant 2 on the left by a constant c_p which depends only on the norm. The main tool in this approach is the notion of a discrete gradient.

Although difficult to prove, Cheeger's bound seems to be less important than the bound of Corollary 3.8. However, the combination of both bounds shows that for every sequence of graphs of bounded degree, their isoperimetric numbers tend to 0 if and only if their second smallest Laplace eigenvalues tend to 0. This observation has an important meaning for the design of "expanding graphs" since it shows that families of "expanders" correspond to families of graphs whose second Laplace eigenvalue is uniformly bounded away from 0. Cf. the notes by Lubotzky [Lu2] in this collection.

Another important observation following from the proof of Theorem 3.10 is that the partition based on the eigenfunction f of λ_2 is not too far from the optimal one since in the proof of the lower bound on M, only the sets V_k $(1 \leq k \leq m)$ have been considered. Constructing partitions based on the eigenfunctions of λ_2 has proved to be one of the most successful heuristics in parallel computation and for divide-and-conquer approach of processor distribution. Several references with evidence about this approach are given in the introduction.

4 Semidefinite programming

4.1 Introduction

At the end of the seventies Khachiyan [Kh] showed how to use the ellipsoid method to derive a polynomial time algorithm for solving linear programs (see also [G-L-S]). After the Karmarkar's algorithm [Karm] appeared in 1984, the field of mathematical programming faced a rapid development. Many new algorithms were introduced and several of them were applied to a more general classes of problems.

Semidefinite programs constitute such a class of problems. A *semidefinite program* is the problem of minimizing a linear function of a variable $x = (x_1, \ldots, x_n)^T \in \mathbf{R}^n$ subject to positive semidefiniteness of a certain matrix $F(x)$. The problem input consists of $c \in \mathbf{R}^n$ and $n+1$ symmetric matrices $F_0, \ldots, F_n \in \mathbf{R}^{m\times m}$ and asks to

$$\begin{array}{ll} \text{minimize} & \langle c, x\rangle \\ \text{subject to} & F(x) \succeq 0 \end{array} \qquad \text{(SP)}$$

where

$$F(x) = F_0 + \sum_{i=1}^{n} x_i F_i \,.$$

The inequality sign in $F(x) \succeq 0$ means that $F(x)$ is a positive semidefinite matrix, i.e., $\langle F(x)z, z\rangle \geq 0$ for all $z \in \mathbf{R}^m$. Let us remark at this point that we will use the fact that for every positive semidefinite matrix F there exists a unique positive semidefinite matrix S such that $F = S^2$. For the obvious reason, the matrix S is denoted by the symbol $F^{1/2}$.

A semidefinite program is a convex optimization problem since its objective function $x \mapsto \langle c, x\rangle$ is a convex function, and the set of feasible solutions is a convex set. This is shown by the next claim.

Claim 4.1 *The feasible region*

$$\mathcal{F} = \{x \in \mathbf{R}^n \mid F(x) \succeq 0\}$$

of the problem (SP) *is a convex set.*

Proof. Suppose that $x, y \in \mathcal{F}$ and take $\lambda \in [0, 1]$. Then for every $z \in \mathbf{R}^m$, we have

$$\langle(\lambda F(x) + (1-\lambda)F(y))z, z\rangle = \lambda\langle F(x)z, z\rangle + (1-\lambda)\langle F(y)z, z\rangle \geq 0\,.$$

Therefore $\lambda F(x) + (1-\lambda)F(y) = F(\lambda x + (1-\lambda)y) \succeq 0$, and hence $\lambda x + (1-\lambda)y \in \mathcal{F}$. □

Let us now show that semidefinite programming is indeed a generalization of linear programming.

Example 4.2 Consider a linear program

$$\begin{array}{ll} \text{minimize} & \langle c, x\rangle \\ \text{subject to} & Ax + b \geq 0 \end{array} \tag{LP}$$

where $c \in \mathbf{R}^n$, $A \in \mathbf{R}^{m\times n}$, and $b \in \mathbf{R}^m$. Since $Ax + b \in \mathbf{R}^m$, the inequality in (LP) denotes componentwise inequality. To formulate (LP) as a semidefinite program, observe first that a vector $x \geq 0$ (componentwise) if and only if $\operatorname{diag}(x) \succeq 0$ (i.e., the diagonal matrix containing components of x on the diagonal is positive semidefinite). Denote by $a_1, \ldots, a_n$ the columns of A. Since

$$\operatorname{diag}(Ax + b) = \sum_{i=1}^{n} x_i \operatorname{diag}(a_i) + \operatorname{diag}(b)\,,$$

the problem (LP) is equivalent to the semidefinite program with $F(x) = F_0 + \sum_{i=1}^n x_i F_i$, where $F_0 = \operatorname{diag}(b)$ and $F_i = \operatorname{diag}(a_i)$, $i = 1, \ldots, n$.

Another important class of semidefinite programs are (convex) quadratically constrained quadratic programs.

Example 4.3 Every convex quadratic function $f : \mathbf{R}^n \to \mathbf{R}$ can be expressed as $f(x) = \langle Ax, x\rangle - \langle b, x\rangle - c$, where $A \in \mathbf{R}^{n\times n}$ is a positive semidefinite matrix, $b \in \mathbf{R}^n$, and $c \in \mathbf{R}$. The eigenvalues of the matrix

$$M = \begin{bmatrix} I & A^{1/2}x \\ (A^{1/2}x)^T & \langle b, x\rangle + c \end{bmatrix}$$

are $\det(M) = -f(x)$ with multiplicity 1, and 1 with multiplicity n. Therefore the constraint $f(x) \leq 0$ is equivalent to $M \succeq 0$. Observe also that M depends affinely on the vector x and can therefore be expressed as

$$M = F_0 + x_1 F_1 + \cdots + x_n F_n$$

with

$$F_0 = \begin{bmatrix} I & 0 \\ 0 & c \end{bmatrix} \quad \text{and} \quad F_i = \begin{bmatrix} 0 & a_i \\ a_i^T & b_i \end{bmatrix}, \quad i = 1, \ldots, n\,,$$

where $a_1, \ldots, a_n$ are the columns of $A^{1/2}$.

A general (convex) quadratically constrained quadratic program (QP) is the following problem:

$$\begin{array}{ll} \text{minimize} & f_0(x) \\ \text{subject to} & f_i(x) \leq 0, \quad i = 1, \ldots, m, \end{array} \tag{QP}$$

where each $f_i : \mathbf{R}^n \to \mathbf{R}$ $(0 \leq i \leq m)$ is a convex quadratic function given by $f_i(x) = \langle A_i x, x\rangle - \langle b_i, x\rangle - c_i$, $A_i \succeq 0$, $b_i \in \mathbf{R}^n$, $c_i \in \mathbf{R}$. By the above, the problem (QP) can be restated as a semidefinite program

$$\begin{array}{ll} \text{minimize} & t \\ \text{subject to} & \begin{bmatrix} I & A_0^{1/2} x \\ (A_0^{1/2} x)^T & \langle b_0, x\rangle + c_0 + t \end{bmatrix} \succeq 0 \\ & \begin{bmatrix} I & A_i^{1/2} x \\ (A_i^{1/2} x)^T & \langle b_i, x\rangle + c_i \end{bmatrix} \succeq 0, \quad i = 1, \ldots, m\,. \end{array}$$

Since a block-diagonal matrix is positive semidefinite if and only if each of its blocks is positive semidefinite, the above $m + 1$ constraints can also be viewed as a single constraint on a large block-diagonal matrix.

Let us remark that it is a standard procedure to introduce an additional variable, in our case t, when transforming a problem into a semidefinite form in order to linearize the objective function and to move its nonlinearity into constraints.

For our applications, the most important semidefinite programs are those for minimizing the largest eigenvalue of an affine combination of symmetric matrices.

EXAMPLE 4.4 Let $A_0, \ldots, A_n \in \mathbf{R}^{m\times m}$ be symmetric matrices, and for $x \in \mathbf{R}^n$, set

$$A(x) = A_0 + \sum_{i=1}^{n} x_i A_i\,.$$

We would like to

$$\begin{array}{ll} \text{minimize} & \lambda_{\max}(A(x)) \\ \text{subject to} & x \in U \end{array}$$

where U is a (linear) subspace of $\mathbf{R}^n$. Similarly as in the previous example, the above problem can be translated into a semidefinite program by introducing an auxiliary variable $t \in \mathbf{R}$:

$$\begin{array}{ll} \text{minimize} & t \\ \text{subject to} & tI - A(x) \succeq 0, \\ & x \in U. \end{array}$$

The first constraint is equivalent to $t \geq \lambda_{\max}(A(x))$. We leave it to the reader to see how both conditions can be combined into a single condition on the positive semidefiniteness of a matrix as required in the standard form of semidefinite programs.

In particular, the bound on the max-cut of a graph stated in Proposition 3.6 is an instance of the problem from Example 4.4, where we take U to be the orthogonal complement of the vector $\mathbf{1}$. Also, the bound on the bipartition width from Corollary 3.4 can be viewed as a semidefinite program of the same form since

$$\max_{x \in U} \lambda_{\min}(A(x)) = \max_{x \in U}\{-\lambda_{\max}(-A(x))\} = -\min_{x \in U} \lambda_{\max}(-A(x))\,.$$

There exist efficient and practically useful algorithms for solving semidefinite programs. Given any $\varepsilon > 0$, the given semidefinite program can be solved within an additive error of ε in polynomial time (where ε is part of the input, its size being proportional to $\log(1/\varepsilon)$). For this purpose one can use the ellipsoid algorithm (cf. [G-L-S]), other polynomial time algorithms for convex programming [Vai], or the interior-point methods [Ali, N-N1, N-N2]. Since the work of Nesterov and Nemirovskii [N-N1], and Alizadeh [Ali] there has been much development in the design and analysis of interior-point methods for semidefinite programming, yielding practically useful algorithms whose performance is comparable, and even superior, to the performance of the simplex method.

4.2 Max-cut and semidefinite programming

Given a (weighted) graph G, the max-cut problem for G can be formulated as a quadratic integer program with variables y_v, $v \in V(G)$:

$$\begin{array}{ll} \text{maximize} & \frac{1}{2} \displaystyle\sum_{uv \in E(G)} a_{uv}(1 - y_u y_v) \\ \text{subject to} & y_v \in \{-1, 1\} \text{ for every } v \in V(G). \end{array} \qquad \text{(MC}_{\text{QI}}\text{)}$$

If y is a feasible solution, then $1 - y_v y_u$ is equal to either 0 or 2. Given a solution y of (MC$_{\text{QI}}$), the set S with the property $\mathrm{mc}(G) = e(S, \bar{S})$ is determined by $S = \{v \in V(G) \mid y_v = 1\}$.

Goemans and Williamson [G-W] considered the following relaxation of (MC$_{\text{QI}}$):

$$\begin{array}{ll} \text{maximize} & \frac{1}{2} \displaystyle\sum_{uv \in E(G)} a_{uv}(1 - \langle z_v, z_u \rangle) \\ \text{subject to} & z_v \in S^{n-1} \text{ for every } v \in V(G). \end{array} \qquad \text{(MC}_{\text{QR}}\text{)}$$

Here, S^{n-1} denotes the $(n-1)$-dimensional sphere in $\mathbf{R}^n$,

$$S^{n-1} = \{x \in \mathbf{R}^n \mid \|x\| = 1\}\,.$$

It is important to observe that the problem (MC$_{\text{QR}}$) can be reformulated as a semidefinite program:

$$\begin{array}{ll} \text{maximize} & \frac{1}{2}\sum_{uv\in E(G)} a_{uv}(1-y_{uv}) \\ \text{subject to} & y_{vv}=1 \text{ for every } v\in V(G) \text{ and} \\ & Y=[y_{uv}]_{u,v\in V(G)} \succeq 0. \end{array} \qquad \text{(MCSP)}$$

CLAIM 4.5 *Problems* (MCQR) *and* (MCSP) *are equivalent.*

PROOF. Denote by Φ_1 and Φ_2 the objective functions of (MCQR) and (MCSP), respectively, and let Φ_1^* and Φ_2^* be the corresponding optimum values. Suppose that $z=\{z_v\in S^{n-1} \mid v\in V(G)\}$ is an optimum solution to (MCQR). Form the matrix $Y=[y_{uv}]_{u,v\in V(G)}$, where $y_{uv}=\langle z_u,z_v\rangle$. This matrix, known as the *Gramm matrix* of vectors z_v ($v\in V(G)$), is easily seen to be positive semidefinite. Clearly, $y_{vv}=1$ for each $v\in V(G)$. Since also $\Phi_1^*=\Phi_1(z)=\Phi_2(Y)$, we have $\Phi_1^*\le\Phi_2^*$.

Conversely, suppose that Y is an optimum solution to (MCSP). Let $z=\{z_v \mid v\in V(G)\}$ be the columns of $Y^{1/2}$. Since $y_{vv}=1$, we have $\langle z_v,z_v\rangle=1$. Therefore z is a feasible solution to (MCQR). Clearly, $\Phi_2(Y)=\Phi_1(z)$, and hence $\Phi_2^*\le\Phi_1^*$. □

Poljak and Rendl [P-R] were the first to realize that the bound of the relaxation (MCSP) is in fact equivalent to the eigenvalue upper bound of Proposition 3.6.

PROPOSITION 4.6 *Let G be a weighted graph of order n. Then the value of an optimum solution to* (MCSP) *is equal to*

$$\frac{n}{4}\cdot\min_c \lambda_{\max}(L(G)+\operatorname{diag}(c))$$

where the minimum is taken over all vectors $c\in\mathbf{R}^V$ with $\sum_{v\in V(G)} c_v=0$.

For a proof (which uses elegant duality theory of semidefinite programs) we refer to [P-R].

Goemans and Williamson suggested the following randomized algorithm based on the relaxation (MCSP) that finds an approximation to the max-cut of G (and also returns the corresponding set $S\subset V(G)$):

ALGORITHM 4.7 (RANDOMIZED MAX-CUT APPROXIMATION ALGORITHM)

Input: *A weighted graph G of order n.*
Output: *A set $S\subseteq V(G)$ and $e(S,\bar S)$.*
1. *Solve the program* (MCSP)*, and let Y be the obtained solution.*
2. *Compute the Cholesky decomposition of $Y=Z^TZ$, and let z_v, $v\in V(G)$, be the columns of Z.*
3. *Choose a random vector $c\in S^{n-1}$ (according to the uniform distribution), and set $S:=\{v\in V(G) \mid \langle c,z_v\rangle\ge 0\}$.*
4. *Compute $e(S,\bar S)$.*
5. *Return S and $e(S,\bar S)$.*

The algorithm can be implemented to run in polynomial time in the size of the input. (Recall that the size of the input depends on n and $\log w(E)$, where $w(E)=\sum_{e\in E(G)} w(e)$.) See [G-W] for more details. In the next section we will learn how one can upgrade Algorithm 4.7 to a deterministic 0.878-approximation algorithm for the max-cut problem.

4.3 Approximating the max-cut

For a weighted graph G with the weight function w, denote by $w(E)$ the sum of the weights $w(e)$ over all edges e of G. Let us first compute the expected value of the weight $e(S, \bar{S})$.

CLAIM 4.8 *Let S be a randomly chosen subset of $V(G)$ where each vertex $v \in V(G)$ belongs to S with probability $\frac{1}{2}$. Then*

$$\mathrm{Exp}[\, e(S, \bar{S})\,] = \frac{1}{2}\, w(E).$$

PROOF. For each $e \in E(G)$, there are exactly 2^{n-1} subsets $S \subseteq V(G)$ such that $e \in E(S, \bar{S})$. Therefore

$$\begin{aligned} \mathrm{Exp}[\, e(S, \bar{S})\,] &= \sum_{S \subseteq V(G)} \frac{1}{2^n} \cdot e(S, \bar{S}) = \frac{1}{2^n} \sum_{S \subseteq V(G)} \sum_{e \in E(S, \bar{S})} w(e) \\ &= \frac{1}{2^n} \sum_{e \in E(G)} 2^{n-1} \cdot w(e) = \frac{1}{2} w(E)\,. \end{aligned}$$

□

It is also easy to describe a deterministic procedure that finds a $\frac{1}{2}$-approximation to $\mathrm{mc}(G)$, i.e., returns a subset $S \subset V(G)$ such that $e(S, \bar{S}) \geq \frac{1}{2}\mathrm{mc}(G)$.

ALGORITHM 4.9 (DETERMINISTIC $\frac{1}{2}$-APPROXIMATION ALGORITHM FOR THE MAX-CUT)

Input: *A weighted graph G.*
Output: *A set $S \subset V(G)$ and $e(S, \bar{S})$ such that $e(S, \bar{S}) \geq \frac{1}{2}\mathrm{mc}(G)$.*

1. *Set $S_1 := \emptyset$ and $S_2 := \emptyset$.*
2. *Take $v \in V(G) \backslash (S_1 \cup S_2)$ and compute $e(\{v\}, S_1)$ and $e(\{v\}, S_2)$.*
3. *If $e(\{v\}, S_1) \geq e(\{v\}, S_2)$, let $S_2 := S_2 \cup \{v\}$.*
   Otherwise, let $S_1 := S_1 \cup \{v\}$.
4. *If $S_1 \cup S_2 \neq V(G)$, goto Step 2.*
5. *Set $S := S_1$ and compute $e(S, \bar{S})$.*
6. *Return S and $e(S, \bar{S})$.*

Note that throughout the algorithm, we have

$$e(S_1, S_2) \geq \frac{1}{2} \sum_{u,v \in S_1 \cup S_2} w(uv)\,,$$

which proves that at the end

$$e(S, \bar{S}) \geq \frac{1}{2}\, w(E) \geq \frac{1}{2}\, \mathrm{mc}(G)$$

holds. There exist examples where the value $e(S, \bar{S})$ returned by Algorithm 4.9 is arbitrarily close to $\frac{1}{2}\mathrm{mc}(G)$.

It is much more difficult to find an α-approximation to $\mathrm{mc}(G)$ for a constant $\alpha > \frac{1}{2}$ in polynomial time. Let us also recall that there exists a constant $\varepsilon > 0$ such that there is no

polynomial time $(1-\varepsilon)$-approximation algorithm for the max-cut problem unless $P = NP$ [P-Y, A-L-M-S-S].

Following [G-W], we will now show that Algorithm 4.7 can be used to find such a 0.878-approximation in polynomial time.

LEMMA 4.10 *The expected weight of the cut $E(S,\bar{S})$ produced by Algorithm 4.7 is equal to*

$$\mathrm{Exp}[\, e(S,\bar{S})\,] = \frac{1}{\pi} \sum_{uv \in E(G)} a_{uv} \arccos\langle z_u, z_v\rangle\,,$$

where z_v, $v \in V(G)$, is an optimum solution of (MCQR).

PROOF. Observe first that

$$\Pr[\, u \in S, v \notin S\,] = \Pr[\, \langle c, z_u\rangle \geq 0, \langle c, z_v\rangle < 0\,] = \frac{\arccos\langle z_u, z_v\rangle}{2\pi}\,.$$

Therefore

$$\begin{aligned}\mathrm{Exp}[\, e(S,\bar{S})\,] &= \sum_{uv\in E(G)} w(uv)\Pr[\, uv \in E(S,\bar{S})\,] = 2\sum_{uv\in E(G)} w(uv)\Pr[\, u\in S, v\notin S\,] \\ &= 2\sum_{uv\in E(G)} w(uv)\frac{\arccos\langle z_u, z_v\rangle}{2\pi} = \frac{1}{\pi}\sum_{uv\in E(G)} w(uv)\arccos\langle z_u, z_v\rangle\,.\end{aligned}$$

□

It is an easy exercise in calculus to show that for $x \in [0,1]$, we have

$$\frac{1}{\pi}\arccos(x) \geq \beta \cdot \frac{1}{2}(1-x)\,, \tag{29}$$

where $\beta = 0.87856$. Therefore Lemma 4.10 implies:

COROLLARY 4.11 *For a weighted graph G, let $E(S,\bar{S})$ be the cut obtained by Algorithm 4.7. Then*

$$\mathrm{Exp}[\, e(S,\bar{S})\,] \geq \beta \cdot \mathrm{mc}(G)\,.$$

PROOF. Lemma 4.10 and inequality (29) imply that

$$\mathrm{Exp}[\, e(S,\bar{S})\,] = \frac{1}{\pi}\sum_{uv\in E(G)} w(uv)\arccos\langle z_u, z_v\rangle \geq \beta\cdot\frac{1}{2}\sum_{uv\in E(G)} w(uv)(1-\langle z_u, z_v\rangle)\,.$$

Since z_v, $v \in V(G)$, is an optimum solution to (MCQR), and since (MCQR) gives an upper bound on $\mathrm{mc}(G)$, we finally get

$$\mathrm{Exp}[\, e(S,\bar{S})\,] \geq \beta \cdot \mathrm{mc}(G)\,.$$

□

It remains to describe how to convert the randomized Algorithm 4.7 into a deterministic one (without substantially increasing its time complexity and without worsening its approximation performance).

Following [G-W], the idea of derandomization is to maintain a set of unit vectors $y_v \in S^m$, $v \in V(G)$, with the property

$$\mathrm{Exp}[\, e(S, \bar{S})\,] \geq \beta \cdot \mathrm{mc}(G)\,, \tag{30}$$

where the partitioning is performed with respect to a random hyperplane in $\mathbf{R}^{m+1}$, and to gradually decrease the dimension m to 0 by transforming y_v, $v \in V(G)$, to a new set of unit vectors $y'_v \in S^{m-1}$, $v \in V(G)$, still having the property (30) (with respect to the partition determined by a random hyperplane in $\mathbf{R}^m$). For $m = 0$, $S^0 = \{-1, 1\}$, and there is only one "random" hyperplane in $\mathbf{R}$. Therefore the final vectors y_v, $v \in V(G)$, determine a set $S := \{v \in V(G) \mid y_v = 1\}$ with the property $e(S, \bar{S}) \geq \beta \cdot \mathrm{mc}(G)$.

Initially, $y_v := z_v \in S^{n-1}$, where z_v, $v \in V(G)$, is an optimum solution to (MCQR). Let us now describe how to decrease the dimension m by 1. Suppose that we have vectors $y_v \in S^m$, $v \in V(G)$, satisfying (30). Decompose S^m into a disjoint union

$$S^m = \bigcup_{\theta \in (-\pi, \pi]} S^m_\theta\,,$$

where

$$S^m_\theta = \{x = (x_1, \ldots, x_{m+1})^T \in S^m \mid x_m = s\cos\theta,\, x_{m+1} = s\sin\theta \text{ for some } s \in \mathbf{R}\}\,.$$

Then there exists an angle θ such that choosing the normal c only from S^m_θ still gives (possibly even stronger) inequality (30). Moreover, such an angle θ can be efficiently computed. For every $v \in V(G)$, let t_v and γ_v be the absolute value and the polar angle of the complex number $x_m + i \cdot x_{m+1}$, respectively. Define

$$y^\circ_v = (y_{v,1}, \ldots, y_{v,m-1}, t_v \cos(\gamma_v - \theta))^T \in \mathbf{R}^m$$

and set

$$y'_v = \frac{y^\circ_v}{\|y^\circ_v\|} \in S^{m-1}\,.$$

It remains to prove that the transition from y_v to y'_v does not violate (30). The key observation that guarantees this is the following:

Claim 4.12 *Suppose that* $x = (x_1, \ldots, x_{m-1}, s\cos\theta, s\sin\theta)^T \in S^m_\theta$. *Let* $x' := (x_1, \ldots, x_{m-1}, s)^T \in S^{m-1}$. *Then*

$$\langle x, y_v\rangle = \langle x', y^\circ_v\rangle\,.$$

Proof. Standard properties of the cosinus give

$$\begin{aligned}\langle x, y_v\rangle - \langle x', y^\circ_v\rangle &= s\cos\theta \cdot t_v \cos\gamma_v + s\sin\theta \cdot t_v \sin\gamma_v - s \cdot t_v \cos(\gamma_v - \theta)\\ &= s \cdot t_v(\,\cos\theta\cos\gamma_v + \sin\theta\sin\gamma_v - \cos(\gamma_v - \theta)) = 0.\end{aligned}$$

□

Consequently, the sign of $\langle x, y_v\rangle$ is the same as the sign of $\langle x', y'_v\rangle$, and therefore the expected value $\mathrm{Exp}[\, e(S, \bar{S})\,]$ of $e(S, \bar{S})$ on S^{m-1} with respect to y'_v, $v \in V(G)$, is the same

as the expectation $\mathrm{Exp}[\, e(S,\bar{S})\,]$ of $e(S,\bar{S})$ on S^m_θ with respect to y_v, $v \in V(G)$, which is in turn at least $\beta \cdot \mathrm{mc}(G)$. This proves that the derandomization works as claimed above.

After the announcement of the approximation algorithm of Goemans and Williamson, semidefinite programming has been successfully applied in the design of a number of other approximation algorithms, for example the max-k-cut (Frieze and Jerrum [F-J]), a 0.931-approximation algorithm for MAX 2-SAT (Feige and Goemans [F-G]), a 0.859-approximation algorithm for MAX DICUT [F-G], and approximate coloring (Karger, Motwani, and Sudan [K-M-S]).

5 Random walks on graphs

Isoperimetric properties and eigenvalues treated in previous sections are closely related to the convergence rates of Markov chains. Several important randomized algorithms discovered in the last decade increased applicability of random walks and Markov chains in solving previously untractable problems. In this section we briefly describe relations between simple random walks in graphs and parameters similar to those treated in previous sections. At the end we mention how these results are used in the design of efficient randomized approximation algorithms. Additional reading on the results related to the presentation in this section can be found, e.g., in [M-R, Kan, Ros, Sin].

5.1 Markov chains

A *Markov chain* consists of a measurable *state space* $\mathcal{V}$, an initial probability distribution (i.e., a probability measure) μ_0 on $\mathcal{V}$, and *transition probabilities* $P(u,\cdot)$ which give, for each state $u \in \mathcal{V}$, a distribution $P(u,\cdot)$ on $\mathcal{V}$ (which represents the probabilities of where the Markov chain will go one step after being in the state u). It is assumed that $u \mapsto P(u,A)$ is a measurable function on $\mathcal{V}$ for each fixed measurable subset $A \subseteq \mathcal{V}$. If $\mathcal{V}$ is a discrete space (in particular, finite), then the initial distribution μ_0 can be specified by the function $x^{(0)} : \mathcal{V} \to \mathbf{R}^+$ such that $\sum_{u\in\mathcal{V}} x^{(0)}_u = 1$. Similarly, the transition probabilities $P(u,v)$ can be described by the *transition matrix* $P = (p_{uv})_{u,v\in\mathcal{V}}$ indexed by $\mathcal{V}$ which has nonnegative real entries $p_{uv} = P(u,\{v\})$ such that for each $u \in \mathcal{V}$, we have $\sum_{v\in\mathcal{V}} p_{uv} = 1$.

Given the initial distribution μ_0 and transition probabilities $P(u,\cdot)$, we can inductively construct distributions μ_t on $\mathcal{V}$, representing the probabilities of where the Markov chain will be after t steps:

$$\mu_t(A) = \int_{\mathcal{V}} P(u,A)\mu_{t-1}(du)\,, \quad t = 1,2,\dots\,. \tag{31}$$

We will be interested only in Markov chains with discrete state space $\mathcal{V}$, which we assume in what follows. In such a case, (31) can be presented more directly as

$$x^{(t)}_v = \sum_{u\in\mathcal{V}} p_{uv} x^{(t-1)}_u \tag{32}$$

or in the matrix form:

$$x^{(t)} = P^T x^{(t-1)} = \cdots = (P^T)^t x^{(0)} \tag{33}$$

where the action of the transpose matrix P^T on the elements of $\mathbf{R}^{\mathcal{V}}$ is determined by the rule of matrix-vector multiplication. The formula (33) is easy to explain informally. It states

that to be in the state v after t steps, we must have been at some state u at step $t-1$ (with probability $x_u^{(t-1)}$), and then jumped from u to v in the next step (with probability p_{uv}).

If the state space $\mathcal{V}$ contains a nonempty proper subset $\mathcal{V}' \subset \mathcal{V}$ such that $P(v, \mathcal{V}') = 1$ for all $v \in \mathcal{V}'$, then the Markov chain is said to be *reducible*. If there is no such subset $\mathcal{V}'$, the Markov chain is *irreducible*. The Markov chain is *periodic*, if the state space $\mathcal{V}$ contains disjoint nonempty subsets $\mathcal{V}_0, \ldots, \mathcal{V}_{d-1}$ ($d \geq 2$) such that $P(u, \mathcal{V}_i) = 1$ for all $u \in \mathcal{V}_{i-1}$ (where the indices are taken modulo d). If there is no such decomposition, the Markov chain is *aperiodic*.

For states $u, v \in \mathcal{V}$ and $t > 0$, let $r_{uv}^{(t)}$ denote the probability that the Markov chain with the initial state u visits the state v for the first time in step t. The probability that the Markov chain with the initial state u visits the state v after some number of steps is denoted by $r_{uv}^{(\infty)}$, i.e.,

$$r_{uv}^{(\infty)} = \sum_{t=1}^{\infty} r_{uv}^{(t)} .$$

A state $v \in \mathcal{V}$ is *transient* if $r_{vv}^{(\infty)} < 1$; otherwise it is *recurrent* (or *persistent*).

The expected number of steps to reach the state v starting from the state u is denoted by h_{uv}. Then

$$h_{uv} = \sum_{t=1}^{\infty} t\, r_{uv}^{(t)} .$$

A *stationary distribution* for the Markov chain with transition matrix P is a probability distribution x such that $x = P^T x$.

The following theorem summarizes the basic properties of finite Markov chains (i.e., Markov chains whose state space $\mathcal{V}$ is finite).

THEOREM 5.1 *Any finite, irreducible, aperiodic Markov chain with the state space $\mathcal{V}$ has the following properties:*

(i) All states $v \in \mathcal{V}$ are aperiodic and recurrent and $h_{vv} < \infty$.

(ii) There is a unique stationary distribution $x^{(\infty)}$, and $x_v^{(\infty)} > 0$ for every $v \in \mathcal{V}$.

(iii) For every $v \in \mathcal{V}$, $r_{vv}^{(\infty)} = 1$ and $h_{vv} = 1/x_v^{(\infty)}$.

(iv) Choose an initial distribution $x^{(0)}$, and let $N(v,t)$ denote the expected number of times the Markov chain visits state v in t steps, i.e., $N(v,t) = \sum_{i=1}^{t} x_v^{(i)}$. Then

$$\lim_{t \to \infty} \frac{N(v,t)}{t} = x_v^{(\infty)} .$$

The proof of Theorem 5.1 is elementary and can be found in most textbooks treating Markov chains. We refer, for example, to [Fe]. The reader can also consult a similar proof of Theorem 5.7.

5.2 Random walks on graphs

Given a (finite) weighted graph G (possibly containing loops), a *random walk* on G is a Markov chain with state space $\mathcal{V} = V(G)$ and with transition probabilities p_{uv} such that $p_{uv} > 0$ if and only if $uv \in E(G)$. The most common rule to assign values to the transition probabilities p_{uv} to step from u to v, which we assume in what follows, is to take

$$p_{uv} = \frac{a_{uv}}{\mathrm{d}_u}\,.$$

This random walk is called the *simple random walk* on G. For the simple random walk on G, the transition matrix $P(G)$ is equal to

$$P(G) = D^{-1}A(G)\,,$$

where $D = \mathrm{diag}(\mathrm{d}_v; v \in V(G))$ is the diagonal matrix with vertex degrees on the diagonal. Although P is not necessarily symmetric, it has only real eigenvalues. This can be seen as follows. Let $L'(G)$ be the *transition Laplacian matrix* of G defined by

$$L'(G) = D^{-1/2}L(G)D^{-1/2}\,.$$

In particular, we have

$$(L'(G))_{uv} = \begin{cases} 1 - \frac{a_{uu}}{\mathrm{d}_u}, & u = v \\ -\frac{a_{uv}}{\sqrt{\mathrm{d}_u \mathrm{d}_v}}, & uv \in E(G) \\ 0\,, & \text{otherwise.} \end{cases} \tag{34}$$

Observe that $L'(G)$ is a symmetric matrix and that for a d-regular graph G, we have

$$L(G) = d \cdot L'(G)\,.$$

Notice also that the difference Laplacian matrix $L(G)$ of G does not change if we add loops to G, while the transition Laplacian matrix $L'(G)$ is changed under addition of loops. We will see that this property can be used to construct graphs with simple random walks that converge rapidly to the stationary distribution.

The transition matrix $P(G)$ of the simple random walk on G can be expressed as follows:

Claim 5.2 $\quad P(G) = I - D^{-1/2}L'(G)D^{1/2}$.

Proof. Since $I - D^{-1/2}L'(G)D^{1/2} = I - D^{-1}L(G)$, the diagonal elements of the matrix are $1 - \mathrm{d}_u^{-1}(L(G))_{uu} = 1 - (\mathrm{d}_u - a_{uu})/\mathrm{d}_u = a_{uu}/\mathrm{d}_u$ $(u \in V(G))$, and the off-diagonal entries are equal to $-\mathrm{d}_u^{-1}(L(G))_{uv} = a_{uv}/\mathrm{d}_u = p_{uv}$ $(u, v \in V(G), u \neq v)$. □

In particular, $I - P(G)$ and $L'(G)$ have the same eigenvalues. Moreover, Claim 5.2 implies that $P(G)$ (and also $P(G)^T$) can be diagonalized, i.e., it has n pairwise orthogonal eigenvectors.

A proof similar to the proof of Proposition 2.8 gives the following result.

CLAIM 5.3 *Let G be a weighted graph with at least two vertices. Then*

$$-1 \le \lambda_{\min}(P(G)) < \lambda_{\max}(P(G)) = 1\,.$$

If G is connected, then $\lambda_{\max}(P(G)) = 1$ is a simple eigenvalue, and we have $\lambda_{\min}(P(G)) = -1$ if and only if G is bipartite.

It is easy to determine, just by looking at the structure of the graph G, whether a random walk on G is aperiodic or irreducible.

CLAIM 5.4 *Let G be a weighted graph. Then:*

(i) The simple (and hence every) random walk on G is periodic if and only if G is bipartite.

(ii) The simple (and hence every) random walk on G is irreducible if and only if G is connected.

The easy proof of Claim 5.4 is left to the reader.

Theorem 5.1 states that for every finite, irreducible, aperiodic Markov chain, there exists unique stationary distribution $x^{(\infty)}$. In case of simple random walks on connected nonbipartite weighted graphs, the distribution $x^{(\infty)}$ can be easily found.

PROPOSITION 5.5 *Let G be a connected, nonbipartite weighted graph. Then the stationary distribution of the simple random walk on G is given by*

$$x_v^{(\infty)} = \frac{\mathrm{d}_v}{2m}, \quad v \in V(G)\,,$$

where $2m = \sum_{v \in V(G)} \mathrm{d}_v$. In particular, if G is d-regular, then the stationary distribution is uniform,

$$x_v^{(\infty)} = \frac{1}{n}, \quad v \in V(G)\,.$$

PROOF. It suffices to check that $x^{(\infty)}$ is an eigenfunction of $P(G)^T$ corresponding to the eigenvalue 1:

$$\begin{aligned} \left(P(G)^T x^{(\infty)}\right)_v &= \sum_{u \in V(G)} P(G)^T_{vu} x_u^{(\infty)} \\ &= \sum_{u \in V(G)} \frac{a_{uv}}{\mathrm{d}_u} \cdot \frac{\mathrm{d}_u}{2m} = \frac{\mathrm{d}_v}{2m} = x_v^{(\infty)}\,. \end{aligned}$$

□

Let us conclude this subsection by an example.

EXAMPLE 5.6 **Card shuffling:** Suppose that a deck of n cards $c_1, \ldots, c_n$ is lying on the table. We would like to shuffle the cards according to the following rule: select randomly i, j $(1 \le i, j \le n)$ and exchange the cards c_i and c_j. To simulate this shuffling process as a simple random walk on a graph, consider the Cayley graph $\mathrm{Cay}(S_n, T)$ of the symmetric group S_n, where T is the set of all transpositions in S_n. Since this graph is bipartite, it is

a standard trick to add a loop to each vertex to avoid the periodicity of the random walk. Denote the obtained graph by G. To assure that our card-shuffling process is faithfully modelled by the simple random walk on G, we have to assign weights to the edges of G appropriately. There are n^2 distinct possibilities to choose the pair i, j: two for each of the $\binom{n}{2}$ transpositions, and n to choose $i = j$ in which case the deck remains unchanged. Therefore we set

$$a_{uv} = \begin{cases} \frac{1}{n}, & u = v \\ \frac{2}{n^2}, & u \neq v. \end{cases} \tag{35}$$

Well, shuffling cards is fun, but we would like to know how long do we have to shuffle so that the cards are properly shuffled. Or, more formally, how fast does the simple random walk on G converge to the stationary distribution? We address this type of questions in the next subsection.

Example 5.6 belongs to a broader class of random walks on groups. Suppose that we have a (finite) group Γ and a symmetric probability distribution p on Γ, i.e., a probability distribution with the property $p(g) = p(g^{-1})$ for every $g \in \Gamma$. Define $S = \{g \in \Gamma \mid p(g) > 0\}$. Then a random walk on Γ is actually a random walk on the graph $G = \mathrm{Cay}(\Gamma, S)$ where the weight of the edge $gh \in E(G)$ is equal to $p(g^{-1}h)$. In particular, since Cayley graphs are regular, the uniform distribution is stationary for any random walk on any (finite) group.

5.3 Rate of convergence of a random walk

As suggested by the results of the previous subsections, there is a close relationship between the eigenvalues of $P(G)$ and the rate of convergence of the simple random walk on G to the stationary distribution.

THEOREM 5.7 *Let G be a connected, nonbipartite weighted graph and $x^{(0)}$ the initial probability distribution on $V(G)$. Set*

$$\lambda = \max\{|\lambda_i(P(G))| \mid \lambda_i(P(G)) \neq 1\}.$$

For the simple random walk on G we have

$$\|x^{(t)} - x^{(\infty)}\| < \lambda^t.$$

PROOF. For $i = 1, \ldots, n$, let $y^{(i)}$ be the eigenfunction of $Q = P(G)^T$ corresponding to the eigenvalue $\lambda_i = \lambda_i(Q) = \lambda_i(P(G))$. We may assume that $\|y^{(i)}\| = 1$ and that $y^{(i)}$, $i = 1, \ldots, n$, are pairwise orthogonal. Recall that $\lambda_n(Q) = 1$ and that the assumptions in theorem imply $\lambda < 1$. Moreover, the Perron-Frobenius theorem shows that all components of $y^{(n)}$ are positive.

Let us write

$$x^{(0)} = \sum_{i=1}^{n} \alpha_i y^{(i)}$$

and observe that $\alpha_n = \langle x^{(0)}, y^{(n)} \rangle \neq 0$. Then

$$x^{(t)} = Q^t x^{(0)} = \sum_{i=1}^{n} \alpha_i \lambda_i^t y^{(i)} = \sum_{i=1}^{n-1} \alpha_i \lambda_i^t y^{(i)} + \alpha_n y^{(n)}.$$

Since $\lambda < 1$, $x^{(t)}$ converges to $\alpha_n y^{(n)} = x^{(\infty)}$. Therefore,

$$\begin{aligned} \|x^{(t)} - x^{(\infty)}\|^2 &= \Big\| \sum_{i=1}^{n-1} \alpha_i \lambda_i^t y^{(i)} \Big\|^2 = \sum_{i=1}^{n-1} \|\alpha_i \lambda_i^t y^{(i)}\|^2 \\ &= \sum_{i=1}^{n-1} \alpha_i^2 \lambda_i^{2t} \|y^{(i)}\|^2 \le \lambda^{2t} \sum_{i=1}^{n-1} \alpha_i^2 \,. \end{aligned}$$

Since also

$$\sum_{i=1}^{n-1} \alpha_i^2 < \sum_{i=1}^{n} \alpha_i^2 = \|x^{(0)}\|^2 \le 1 \,,$$

we finally get $\|x^{(t)} - x^{(\infty)}\| < \lambda^t$. □

EXAMPLE 5.8 Let us consider the random walk on the d-dimensional hypercube Q_d. Note that Q_d is a Cayley graph of the group $\mathbf{Z}_2^d$. Since Q_d is bipartite, we add a loop to each vertex, and denote the obtained graph by G. We would like to assign the weights to the loops and proper edges of G in such a way that λ becomes as small as possible. Let α be the weight assigned to the loops and β the weight of the proper edges of G. We also require $\alpha + d\beta = 1$. Then

$$P(G) = \alpha I + \beta A(Q_d)$$

where $A(Q_d)$ is the adjacency matrix of Q_d. Example 2.5 shows that the eigenvalues of $P(G)$ are $\alpha + \beta(d - 2i)$, $i = 0, \ldots, d$, where the multiplicity of $\lambda_i = \alpha + \beta(d - 2i)$ is equal to $\binom{d}{i}$. Therefore

$$\lambda = \max\{\alpha + \beta(d-1), |\alpha - \beta d|\} \,.$$

By balancing both terms, we get equality when $\alpha = \beta = \frac{1}{d+1}$. Hence

$$\lambda = \frac{d-1}{d+1} = 1 - \frac{2}{d+1} \,.$$

By Theorem 5.7, the rate of convergence can be estimated by

$$\lambda^t = \left(\frac{d-1}{d+1}\right)^t = \left(1 - \frac{2}{d+1}\right)^t \le \exp\Big(-\frac{2t}{d+1}\Big) \,.$$

Let us remark that similar estimates can be established for other Abelian groups (cf., e.g., [Ros]).

EXAMPLE 5.9 **Card shuffling:** In this case, general analysis is more complicated than for the d-cube since it involves group representations of S_n. In the special case of Example 5.6 we obtain

$$\lambda = 1 - \frac{2}{n} \le \exp(-2/n) \,,$$

and consequently

$$\|x^{(t)} - x^{(\infty)}\| \le \exp(-\frac{2t}{n}) \,.$$

See [D-Sa] for more details.

EXAMPLE 5.10 **Usual card shuffling:** This problem was considered by Bayer and Diaconis [B-D]. They showed that $\frac{3}{2}\log_2 n$ iterations are enough (and also necessary) for good card shuffling of the deck of n cards. An interesting result of their analysis of the rate of convergence of random walks on S_n corresponding to card shuffling is the cut-off phenomenon which states that n cards become "well shuffled" (with high probability) all of the sudden in a very short period at the time $\frac{3}{2}\log_2 n + o(\log_2 n)$. In particular, 7 ordinary "riffle" shuffles are (required and) enough to properly mix the ordinary deck of 52 cards. For additional background see [Di].

Perhaps the most useful distance between probability distributions x, y of the Markov chain is the so-called "chi-squared" distance which is defined as follows:

$$\chi^2(x,y) = \sum_{v \in V(G)} \frac{(x_v - y_v)^2}{y_v}\,.$$

Obviously, the definition makes sense only when $y_v > 0$ for every $v \in V(G)$. A proof similar to the proof of Theorem 5.7 gives:

THEOREM 5.11 *For the simple random walk on a non-bipartite weighted graph we have*

$$\chi^2(x^{(t)}, x^{(\infty)}) \le \lambda^t \cdot \chi^2(x^{(0)}, x^{(\infty)}).$$

The quantity

$$\frac{1}{1-\lambda}$$

is called the *mixing time* of the random walk and is obviously of interest since the above theorem implies that in this many steps, the chi-squared distance to the stationary distribution $x^{(\infty)}$ is cut by a constant factor.

The quantity $1-\lambda$ is related to the second smallest eigenvalue $\lambda_2(I-P)$ which is the same as the second smallest eigenvalue of the transition Laplace matrix $L'(G)$.

The isoperimetric constant related to the transition Laplacian is also known as *conductance* of the corresponding Markov chain (cf., e.g., [Sin]). In case of the simple random walk on the graph G, the conductance is defined as

$$i_P(G) = \min\left\{ \frac{\sum_{u\in S}\sum_{v\notin S} p_{uv}\mathrm{d}_u}{\mathrm{d}(S)} \;\middle|\; S \subset V(G), 0 < \mathrm{d}(S) \le m \right\}$$

where

$$\mathrm{d}(S) = \sum_{v\in S} \mathrm{d}_v \quad \text{and} \quad m = \frac{1}{2}\sum_{v\in V} \mathrm{d}_v = \frac{1}{2}\mathrm{d}(V).$$

If the graph G is regular, then the conductance coincides with the isoperimetric number of G (divided by the degree).

Similar proofs as given in Section 3 (for Corollary 3.8 and Theorem 3.10) give the following bounds:

THEOREM 5.12 *For the simple random walk on the graph G we have*

$$\frac{1}{2}\, i_P^2(G) \le \lambda_2(I-P) = \lambda_2(L'(G)) \le 2\, i_P(G).$$

For proofs we refer, for example, to [Mo1, Mo4].

Since $\lambda_2(I-P) \ge 1-\lambda$, Theorem 5.12 gives a bound on the mixing time as well.

5.4 Some applications

Rapidly mixing Markov chains proved to be an important tool in the design of polynomial time randomized algorithms. In what follows, we will describe two such applications, and we refer the reader to [M-R, Kan, Ros] for additional applications and for more detailed presentation.

First we describe an application which concerns computing an approximation of the volume of a convex body. Suppose that the convex body $K \subseteq \mathbf{R}^n$ is given by the *membership oracle*, i.e., for each point $x \in \mathbf{R}^n$, one can decide in constant (or polynomial) time if $x \in K$ or not. Bárány and Füredi [B-F] proved that an approximation V for the volume of K such that

$$\frac{1}{2}\,\mathrm{Vol}(K) < V < 2\mathrm{Vol}(K)$$

(or even with 2 being replaced by a polynomial function in n) cannot be computed in polynomial time. See also [L-S1, L-S2]. However, Dyer, Frieze, and Kannan [D-F-K] found a polynomial time randomized approximation algorithm for computing the volume of the convex set K based on sampling random points in K. Lovász and Simonovits [L-S1, L-S2] improved their algorithm by providing random walk sampling with better mixing and by proving better isoperimetric estimates. Further improvements have been obtained since; cf. [Kan].

The basic idea of the randomized algorithms for approximating the volume of the convex body K is as follows. Let B be a ball contained in K. (Usually, such a ball is part of the input.) The algorithm constructs a sequence of convex bodies $K_0 = B \subset K_1 \subset \cdots \subset K_t = K$ such that:

(i) There is a constant $c > 0$ such that for $i = 1, \ldots, t$, we have

$$\mathrm{Vol}(K_i) \leq c \cdot \mathrm{Vol}(K_{i-1})\,.$$

(ii) The length t of the sequence is polynomial in n.

In such a situation, it suffices to construct a fully polynomial randomized approximation scheme that estimates the ratio

$$\frac{\mathrm{Vol}(K_i)}{\mathrm{Vol}(K_{i-1})} \qquad (i = 1, \ldots t)\,.$$

The idea is to choose a random point in K_i and check whether it also belongs to K_{i-1}. Property (i) guarantees that such an approach works. The nontrivial part of this procedure is to choose a random point in K_i. This is done by imposing a suitably fine grid over K_i and performing a random walk on the vertices of the grid. The crucial step in the method is to prove that the random walk is rapidly mixing: in a number of steps that is polynomial in n, the probability distribution of the walk becomes almost uniform on all vertices of the grid. The reader is invited to consult [D-F-K, L-S1, L-S2] for details.

Another application, in a way similar to the first one, deals with approximate counting of perfect matchings in a (bipartite) graph (and therefore also with the approximation of the permanent of a 01-matrix). Let us recall that computing the permanent of a 01-matrix is $\#P$-hard [Val]. Each 01-matrix A of size $n \times n$ determines a bipartite graph G on $n + n$

vertices in which the ith vertex in the first bipartition class is adjacent to the jth vertex in the second class if and only if $a_{ij} = 1$. Then $\mathrm{per}(A)$ is equal to the number of perfect matchings of G. Broder [Bro] proposed the following Markov chain approach to approximating the number of perfect matchings of G.

One starts with a bipartite graph G on $n+n$ vertices having at least one perfect matching. The state space $\mathcal{V}$ of the Markov chain is the set of all perfect and all near-perfect matchings. (The matching is said to be *near-perfect* if it covers all vertices but one in each bipartition class of the graph.) We start by an arbitrary matching $M \in \mathcal{V}$. The transitions in the Markov chain are as follows. Let M be the current state. We stay with probability 1/2 in the same state, and with probability 1/2 we do the following. Pick an edge $e = uv$ of G uniformly at random and:

(a) If M is a perfect matching and $e \in M$, then move to $M \backslash \{e\}$.

(b) If M is a near-perfect matching and no edge of M contains u or v, then move to the matching $M \cup \{e\}$.

(c) If M is a near-perfect matching, an edge uw incident with u is in M, and no edge of M contains v, then move to $(M \cup \{e\}) \setminus \{uw\}$.

(d) In all other cases stay at M.

Jerrum and Sinclair [J-S, S-J] proved (by estimating the isoperimetric number) that this random walk mixes rapidly if the graph is "dense enough" (e.g., if each row and column of A contains at least $n/2$ ones). This yields a polynomial time randomized approximation algorithm for computing the number of perfect matchings of "dense" bipartite graphs. For details, the reader is invited to consult [J-S] or [Sin].

6 Infinite graphs

In this section we show how to extend the results of previous sections to infinite locally finite graphs. Most of the results can be derived for weighted graphs where the local finiteness condition is replaced by the requirement that $\mathrm{d}_v < \infty$ for each $v \in V(G)$. However, some results, for instance those about the growth, do not extend to the weighted case.

In considering the appropriate notions of infinite graphs there is a possibility of introducing the *essential graph invariants*, examples of which are presented in Subsection 6.1. In Subsection 6.2 we introduce the Laplace matrix and the Laplace spectrum of infinite graphs and prove some counterparts to the results of Section 3. In the last subsection we touch the concepts of amenability and transience of graphs. A thorough treatment of these results can be found in [Mo4] whose presentation is partially followed also in this section.

6.1 Essential invariants of infinite graphs

Graphs G and H are said to be *equivalent* (*by finite*) or *almost isomorphic* if there is a bijection $\psi : V(G) \to V(H)$ which maps adjacent, or non-adjacent pairs of vertices of G to adjacent and non-adjacent pairs in H, respectively, with finitely many exceptions. Equivalently, H can be obtained from G by first deleting and then adding finitely many edges, up to an isomorphism.

We shall denote by $\Delta(G)$ and $\delta(G)$ the maximum and minimum vertex degree in G, respectively. It is possible that $\Delta(G) = \infty$. These numbers have their "essential" counterparts, the *essential maximum degree* $\Delta'(G)$ and the *essential minimum degree* $\delta'(G)$, defined by

$$\Delta'(G) := \inf \{\Delta(H) \mid H \text{ equivalent to } G\}$$

and

$$\delta'(G) := \sup \{\delta(H) \mid H \text{ equivalent to } G\} .$$

It may happen that $\Delta'(G) = \infty$ and $\delta'(G) = \infty$. Clearly, $\Delta'(G)$ is equal to the minimal value d for which there are only finitely many vertices of G of degree $> d$. Similarly, $\delta'(G)$ is the minimal d with infinitely many vertices of degree d. It is obvious that $\delta'(G) \leq \Delta'(G)$. These two quantities are defined in such a way that no finite perturbation of G changes their values, i.e., if G and H are equivalent then $\Delta'(G) = \Delta'(H)$ and $\delta'(G) = \delta'(H)$. Graph invariants with this property are said to be *essential*. So, $\Delta'(G)$ and $\delta'(G)$ are the first examples of essential graph invariants we met.

Let $v \in V(G)$. Denote by $B_n(v)$ the set of all vertices of G at distance at most n from v (the *ball* of radius n centred at v), and let $b_n(v) := |B_n(v)|$. If necessary to expose the graph, we write $b_n(G, v)$ and $B_n(G, v)$. The graph G has *exponential growth* (from the vertex v) if $b_n(v) \geq Cq^n$ for some constants $C > 0$, $q > 1$, and each $n \geq 0$. It has *polynomial growth* if $b_n(v) \leq p(n)$ where $p(.)$ is a polynomial. G has *subexponential growth* if it does not grow exponentially. Note that the type of the growth is independent of v if G is connected. Let

$$\varepsilon(G, v) := \limsup_{n\to\infty} (b_n(G, v))^{1/n}$$

and

$$\tau(G, v) := \liminf_{n\to\infty} (b_n(G, v))^{1/n} .$$

If v and u are vertices in the same component of G, then $b_n(u) \leq b_{n+d}(v) \leq b_{n+2d}(u)$ where $d = \text{dist}(u, v)$. It follows that $\varepsilon(G, v)$ and $\tau(G, v)$ are constant on each component of the graph. Define

$$\varepsilon(G) := \sup \{\varepsilon(G, v) \mid v \in V(G)\}$$

and

$$\tau(G) := \sup \{\tau(G, v) \mid v \in V(G)\} .$$

By the above conclusion, the suprema might be taken on representatives of each of the connected components only.

LEMMA 6.1 *If e is an edge of the graph G, then $\varepsilon(G - e) = \varepsilon(G)$ and $\tau(G - e) \leq \tau(G)$. If e is not a cutedge then $\tau(G - e) = \tau(G)$.*

PROOF. The proof of $\varepsilon(G - e) = \varepsilon(G)$ can be found in [Mo1]. To verify the relations for τ, let $e = uv$. Clearly, $\tau(G, v) \geq \tau(G - e, v)$ and $\tau(G, v) = \tau(G, u) \geq \tau(G - e, u)$. Consequently, $\tau(G) \geq \tau(G - e)$. Assume now that e is not a cutedge. Then u and v belong to the same component of $G - e$. Let d be the distance between u and v in $G - e$. Clearly, $b_n(G, v) \leq b_{n+d}(G - e, v)$. Therefore $\tau(G, v) \leq \tau(G - e, v)$. The same holds for u instead of v. This implies that $\tau(G) \leq \tau(G - e)$, so by the converse inequality proved above, $\tau(G) = \tau(G - e)$. □

It may happen that $\tau(G-e) < \tau(G)$. There are also cases where $\tau(G) > 1$ and $\tau(G-e) = 1$. Examples are not hard to construct.

COROLLARY 6.2 *The numbers $\varepsilon(G)$ and $\tau'(G) := \inf\{\tau(H) \mid H$ equivalent to $G\}$ are essential graph invariants.*

PROOF. ε is essential by Lemma 6.1, since addition or deletion of edges does not affect its value. On the other hand, τ' is essential since for G and G' equivalent, the set of graphs which are equivalent to G is equal to the equivalence class of G'. □

PROPOSITION 6.3 *Let G be a graph and $v \in V(G)$. Then $\tau(G,v) > 1$ if and only if G has exponential growth at v.*

PROOF. First, if $b_n(v) \geq Cq^n, q > 1, C > 0$, then $\tau(G,v) \geq q > 1$. Conversely, if $\tau(G,v) > 1$, then for an arbitrarily small $\alpha > 0$,

$$b_n(v)^{1/n} \geq \tau(G,v) - \alpha \tag{36}$$

for all but finitely many values of n. Take $\alpha := \frac{1}{2}(\tau(G,v)-1)$ and $q := \tau(G,v) - \alpha > 1$. By (36), $b_n(v) \geq q^n$ for all but finitely many n, thus $b_n(v) \geq Cq^n$ for some $C > 0$ and for each n. □

The *isoperimetric number* $i(G)$ of G is the number

$$i(G) := \inf\left\{\frac{e(S,\bar{S})}{|S|} \;\Big|\; S \subset V(G),\, 0 < |S| < \infty\right\}.$$

The *essential isoperimetric number* of G is

$$i'(G) := \sup\ \{i(G') \mid G' \text{ equivalent to } G\}\ .$$

It is clear that $i'(G) \geq i(G)$. It is also immediate that $i(G) \leq \delta(G)$ and $i'(G) \leq \delta'(G)$. However, these inequalities need not be very tight since there are examples where $i'(G) = 0$ and $\delta'(G) = \infty$. On the other hand,

$$i'(G) \leq \Delta'(G) - 2. \tag{37}$$

This can be shown as follows. Let G' be equivalent to G. Then it has only finitely many vertices of degree greater than $\Delta'(G)$. Therefore one can find an arbitrarily large finite $S \subset V(G')$ such that all vertices in S have degree at most $\Delta'(G)$ in G', and the subgraph of G' induced on S is connected. Then, in G',

$$e(S,\bar{S}) \leq \Delta'(G)\cdot|S| - 2e(S,S) \leq \Delta'(G)|S| - 2(|S|-1)\ ,$$

which implies (37). This bound is best possible since for the Δ-regular tree T_Δ, $i(T_\Delta) = i'(T_\Delta) = \Delta - 2$.

THEOREM 6.4 *Let G be a connected locally finite graph with $\Delta'(G) < \infty$. Then*

$$i(G) \le i'(G) \le \Delta'(G)\frac{\tau(G)-1}{\tau(G)+1} \ . \tag{38}$$

PROOF. The first inequality is obvious. By Lemma 6.1, $\tau(G)$ does not change after adding finitely many edges to G since G is connected. Thus we may assume that $i(G)$ is arbitrarily close to $i'(G)$, and so it is sufficient to show that

$$i(G) \le \Delta'(G) \cdot \frac{\tau(G)-1}{\tau(G)+1} \ . \tag{39}$$

Choose a vertex $v \in V(G)$ and let $s_n := b_n(v) - b_{n-1}(v)$. For n large enough, all vertices at distance n from v have degree at most $\Delta'(G)$. Hence

$$\begin{aligned} \Delta'(G)s_{n+1} &\ge e(B_{n+1}, V\backslash B_{n+1}) + e(B_n, V\backslash B_n) \\ &\ge i(G)(b_{n+1}+b_n) = i(G)(2b_n + s_{n+1}). \end{aligned}$$

It follows that $(\Delta'(G) - i(G))s_{n+1} \ge 2i(G)b_n$ and hence

$$b_{n+1} = b_n + s_{n+1} \ge b_n \frac{\Delta'(G)+i(G)}{\Delta'(G)-i(G)}$$

for n large enough. Therefore

$$b_n \ge C \cdot \left(\frac{\Delta'(G)+i(G)}{\Delta'(G)-i(G)}\right)^n$$

for some $C > 0$ and each $n \ge 1$. So $\tau(G) \ge (\Delta'(G)+i(G))/(\Delta'(G)-i(G))$. This is equivalent to (39). □

COROLLARY 6.5 *If $\Delta'(G) < \infty$ and $i'(G) > 0$, then $\tau(G) > 1$, and so G has exponential growth in some of its components.*

There are graphs with exponential growth and with $i'(G) = 0$. For example, Cayley graphs of some soluble groups which are not nilpotent by finite are known to grow exponentially but having $i'(G) = 0$, see [Ro]. On the other hand, there are graphs with $\Delta'(G) = \infty$ and $i'(G) > 0$ and having polynomial growth. Take, for example, the graph whose vertices are all integers, and between i and $i+1$ there are $|i|+1$ parallel edges, $-\infty < i < +\infty$. This graph is easily seen to have $i(G) = i'(G) = 1$, but it grows linearly. If we want simple graphs, we may add a vertex of degree two on each edge, or replace each vertex i by a clique of order $|i|+1$, and between any two consecutive cliques put a complete join. This shows that the assumptions in Corollary 6.5 cannot be omitted.

There are other possibilities to define isoperimetric constants of graphs, by taking other distances in graphs. The *transition isoperimetric number* $i_P(G)$ is defined as follows. If G is a graph with no edges, then we set $i_P(G) = 0$. Otherwise

$$i_P(G) := \inf\left\{\frac{e(S,\bar{S})}{\mathrm{d}(S)} \;\middle|\; S \subset V(G), \mathrm{d}(S) \ne 0, |S| < \infty\right\}$$

where $\mathrm{d}(S) := \sum_{v \in S} \mathrm{d}_v$ is the sum of the degrees of the vertices in S. Clearly, $0 \le i_P(G) < 1$. In contrast to $i(G)$, the transition isoperimetric number does not properly measure the connectivity of the graph since it may happen that adding an edge to a graph decreases its value. It is easily seen that $\delta(G) i_P(G) \le i(G) \le \Delta(G) i_P(G)$. Therefore $i_P(G)$ has advantage over $i(G)$ in case $\Delta(G) = \infty$ only. The *essential transition isoperimetric number* $i'_P(G)$ is equal to the supremum of all $i_P(G')$, where G' is equivalent by finite to G. A similar result as Theorem 6.4 holds for $i_P(G)$.

THEOREM 6.6 *Let G be a connected locally finite graph. Then:*

(a) Regardless of the degrees in G,

$$\tau(G) \ge \sqrt{\frac{1 + i'_P(G)}{1 - i'_P(G)}}\ , \quad i.e., \quad i_P(G) \le i'_P(G) \le \frac{\tau^2(G) - 1}{\tau^2(G) + 1}\ . \tag{40}$$

(b) For a vertex $v \in V(G)$, let D_n be the maximum degree of vertices at distance n from v. If $\limsup_{n \to \infty} D_n^{1/n} = 1$ then

$$\tau(G) \ge \frac{1 + i'_P(G)}{1 - i'_P(G)}\ , \quad i.e., \quad i_P(G) \le i'_P(G) \le \frac{\tau(G) - 1}{\tau(G) + 1}\ . \tag{41}$$

(c) If there is a constant $M < \infty$ such that each vertex of G is contained in at most M edge-disjoint cycles, then (41) holds.

For a proof we refer to [Mo4].

COROLLARY 6.7 *If $i'_P(G) > 0$, then $\tau(G) > 1$, and so G has exponential growth in some of its components.*

6.2 The Laplace spectrum of infinite graphs

We define the Laplace matrix $L(G)$ of an infinite locally finite graph G in the same way as for finite graphs.

Let $\ell^2(V)$ denote the Hilbert space of all functions $f : V \to \mathbf{R}$ such that

$$\|f\|^2 = \sum_{v \in V} |f_v|^2 < \infty\ .$$

The inner product in $\ell^2(V)$ is defined as $\langle x, y \rangle = \sum_{v \in V} f_v g_v$. The Laplace matrix $L(G)$ acts naturally on $\ell^2(V)$ as a linear operator. In the following it will be assumed that $\Delta(G) < \infty$. This condition implies that $L(G)$ determines a bounded self-adjoint linear operator on $\ell^2(V)$. Its spectrum $\sigma_L(G)$ is real and (cf., e.g., [M-W])

$$\sigma_L(G) \subseteq [0, 2\Delta(G)]\,.$$

The reader is referred to [M-W] for more details about the spectra of infinite graphs.

There is an alternative way of defining $\sigma_L(G)$ since the spectrum of $L(G)$ is the *approximate point spectrum* in $\ell^2(V)$. This means that $\lambda \in \sigma_L(G)$ if and only if there is a sequence of (not necessarily distinct) unit[1] functions $f^{(n)}$ $(n = 1, 2, 3, \ldots)$ such that

$$\|L(G)f^{(n)} - \lambda f^{(n)}\| \to 0 \ , \qquad \text{as} \quad n \to \infty \ .$$

The number λ is an *eigenvalue* of L if there exists a function $f \in \ell^2(V)$ such that $Lf = \lambda f$. The dimension of the *eigenspace* $\{f \in \ell^2(V) \mid Lf = \lambda f\} \subseteq \ell^2(V)$ is called the *multiplicity* of λ.

The value related to the second smallest eigenvalue of finite graphs is the infimum of $\sigma_L(G)$:

$$\lambda_1(G) := \inf \sigma_L(G).$$

It can be expressed as

$$\lambda_1(G) = \inf \left\{ \frac{\langle L(G)f, f\rangle}{\langle f, f\rangle} \ \Big| \ f \in \ell^2(V), f \neq 0 \right\}. \tag{42}$$

The "essential" invariant corresponding to the spectrum is the *essential spectrum* of $L(G)$. The essential spectrum of a self-adjoint linear operator B on a Hilbert space consists of all those elements in the spectrum of B which are not isolated eigenvalues of finite multiplicity. It is well-known (cf., e.g., [Kat, §X.2]) that these are exactly those $\lambda \in \sigma(B)$ which remain in the spectrum whenever B is changed by a compact perturbation, i.e., $\lambda \in \sigma(B + K)$ for every compact linear operator K. It follows that the essential spectrum is an essential graph invariant since equivalence by finite perturbs the graph matrices in finitely many entries only and thus presents only compact perturbations. The elements of the essential spectrum are also characterized as the approximate eigenvalues of infinite multiplicity [F-S-W] (cf. also [Kat]). This means that λ is in the essential spectrum of B if and only if there are *pairwise orthogonal* unit functions $f^{(n)}$, $n = 1, 2, 3, \ldots$, such that

$$\|Bf^{(n)} - \lambda f^{(n)}\| \to 0 \ , \qquad \text{as} \quad n \to \infty \ .$$

We shall denote by $\lambda_1'(G)$ the infimum of the essential spectrum of $L(G)$. Clearly, $\lambda_1(G) \leq \lambda_1'(G)$. Later we shall need the following inequality:

$$\lambda_1'(G) \leq \frac{\Delta'(G) + \delta'(G)}{2} - 1 < \Delta'(G) \tag{43}$$

if $\delta'(G) \geq 1$. Its proof goes as follows. There are infinitely many pairs u_i, v_i of adjacent vertices, such that $\deg(u_i) \leq \delta'(G)$ and $\deg(v_i) \leq \Delta'(G)$. Let $g^{(1)}, g^{(2)}, \ldots$ be their normalized characteristic functions (i.e., $g^{(i)}_{v_i} = g^{(i)}_{u_i} = \frac{1}{\sqrt{2}}$, and $g^{(i)}_v = 0$ at other vertices v). Then

$$\langle L(G)g^{(i)}, g^{(i)}\rangle \leq \frac{1}{2}(\mathrm{d}_{u_i} + \mathrm{d}_{v_i} - 2) \leq \frac{\Delta'(G) + \delta'(G)}{2} - 1.$$

Since this happens for infinitely many pairwise orthogonal unit functions $g^{(i)}$, an element of the essential spectrum must be $\leq \frac{\Delta'(G)+\delta'(G)}{2} - 1$. The last conclusion is proved as follows.

[1] A function $f \in \ell^2(V)$ is called a *unit* function if $\|f\| = 1$.

We claim that if $\langle Lf^{(i)}, f^{(i)}\rangle \le t$ for infinitely many pairwise orthogonal unit functions $f^{(i)}$, then there is some $\lambda \le t$ in the essential spectrum of L. It is known [St] that for some compact symmetric operator K, the spectrum of $L+K$ is equal to the essential spectrum of L. Since K is compact, $\langle Kf^{(i)}, f^{(i)}\rangle \to 0$ as $i \to \infty$. Consequently

$$\begin{aligned}\lambda_1'(L) &= \lambda_1(L+K) = \inf\{\langle (L+K)f, f\rangle \mid \|f\| = 1\} \\ &\le \inf\{\langle Lf^{(i)}, f^{(i)}\rangle + \langle Kf^{(i)}, f^{(i)}\rangle\} \le t.\end{aligned}$$

THEOREM 6.8 *Let G be a locally finite graph, let $\Delta = \Delta(G) < \infty$, and let $\Delta' = \Delta'(G)$. Then*

$$i(G) \ge \lambda_1(G)\frac{\Delta^2}{\Delta^2 - \Delta - \lambda_1(G)} \ge \lambda_1(G) \tag{44}$$

and

$$i'(G) \ge \lambda_1'(G)\frac{\Delta'^2}{\Delta'^2 - \Delta' - \lambda_1'(G)} \ge \lambda_1'(G)\ . \tag{45}$$

PROOF. Let U be an arbitrary finite subset of $V = V(G)$. Define $f \in \ell^2(V)$ by setting $f_v = 1$ if $v \in U$, and otherwise $f_v = \frac{1}{\Delta} n_v$, where n_v is the number of edges joining v to vertices in U. Denote by W the set of those vertices of $V \setminus U$ which have a neighbor in U. By (42),

$$\lambda_1(G)\|f\|^2 \le \langle L(G)f, f\rangle\ . \tag{46}$$

Similarly as in the finite case we have

$$\langle L(G)f, f\rangle = \sum_{uv \in E(G)} (f_u - f_v)^2\,. \tag{47}$$

Since $f_u - f_v$ is non-zero only if v or u lies in W, we get from (46) and (47):

$$\begin{aligned}\lambda_1\|f\|^2 &= \lambda_1\Big(|U| + \sum_{v\in W}\frac{n_v^2}{\Delta^2}\Big) \le \sum_{vu\in E(G)} (f_u - f_v)^2 \\ &\le \sum_{v\in W}\Big(n_v\Big(1 - \frac{n_v}{\Delta}\Big)^2 + (\Delta - n_v)\Big(\frac{n_v}{\Delta}\Big)^2\Big) \\ &= \sum_{v\in W} n_v - \sum_{v\in W}\frac{n_v^2}{\Delta} = e(U, \bar{U}) - \frac{1}{\Delta}\sum_{v\in W} n_v^2\,.\end{aligned} \tag{48}$$

By rearranging this inequality and using the fact $n_v^2 \ge n_v$, one immediately gets

$$e(U,\bar{U}) - \lambda_1|U| \ge \frac{\Delta + \lambda_1}{\Delta^2}\sum_{v\in W} n_v \ge \frac{\Delta + \lambda_1}{\Delta^2} e(U, \bar{U}).$$

It follows that

$$\frac{e(U,\bar{U})}{|U|} \ge \lambda_1 \frac{\Delta^2}{\Delta^2 - \Delta - \lambda_1}$$

which implies (44) since U was arbitrary.

The proof of (45) needs more care. Fix an arbitrarily small $\varepsilon > 0$. First we shall prove that there exists a graph G_1, which can be obtained from G by adding finitely many edges, such that $\lambda_1(G_1) \ge \lambda_1'(G) - \varepsilon$.

The only elements in the Laplacian spectrum of G which are smaller than $l = \lambda_1'(G)$ are isolated eigenvalues of finite multiplicity. Let N be the span of the eigenspaces of all those eigenvalues of $L(G)$ which are smaller than $l - \frac{\varepsilon}{2}$, and let $n := \dim N < \infty$. Fix an orthonormal basis $f^{(1)}, f^{(2)}, \ldots, f^{(n)}$ of N. It should be mentioned at once that for any $f \in \ell^2(V)$ which is orthogonal to N

$$\langle L(G)f, f\rangle \geq (l - \frac{\varepsilon}{2})\|f\|^2 \ . \tag{49}$$

Let U be a finite subset of $V(G)$ such that for each $i = 1, 2, \ldots, n$,

$$\sum_{u\in U} \left(f_u^{(i)}\right)^2 > 1 - \delta \ , \qquad \text{i.e.,} \quad \sum_{u\notin U} \left(f_u^{(i)}\right)^2 < \delta \ , \tag{50}$$

where $\delta > 0$ is a small number to be fixed later (it will depend on ε, n, G).

Let G_1 be the graph which is obtained from G by adding, for each vertex $u \in U$, m edges joining u to m new distinct neighbors which lie out of U. Denote by $L_1 := L(G_1)$ its Laplacian matrix. We shall prove that $\lambda_1(G_1) \geq l - \varepsilon$, assuming m is large enough. Note that m may depend on ε, n, and G.

Take an arbitrary $f \in \ell^2(V)$, $\|f\| = 1$. We shall prove that $\langle L_1 f, f\rangle \geq l - \varepsilon$ which will imply, by (42), that $\lambda_1(G_1) \geq l - \varepsilon$. It is easy to see that we may assume that $f_v \geq 0$ for each $v \in V(G)$ (apply, for example, (47)). Write now $f = g + h$ where g agrees with f on U, and h agrees with f at other coordinates.

If $\|g\|^2 \leq \delta$, then we do the following calculation. Let $f = p+q$ where $p \in N$ and $q \perp N$. By (49), $\langle Lq, q\rangle \geq (l - \frac{\varepsilon}{2})\|q\|^2$, while $\langle Lp, p\rangle$ can be estimated as follows. If $p = \sum_{i=1}^n \alpha_i f^{(i)}$, then $\|p\|^2 = \sum_{i=1}^n |\alpha_i|^2$ and

$$|\alpha_i| = |\langle f, f^{(i)}\rangle| = \sum_{u\in U} f_u f_u^{(i)} + \sum_{v\notin U} f_v f_v^{(i)} < \|g\| + \|f\|\sqrt{\delta} \leq 2\sqrt{\delta} \ . \tag{51}$$

In the last inequality we applied the Cauchy-Schwartz inequality and (50). Consequently, $\|p\|^2 < 4n\delta = \frac{\varepsilon}{2\Delta(G)}$ if we choose $\delta := \frac{\varepsilon}{8n\Delta(G)}$. Therefore $\|q\|^2 = \|f\|^2 - \|p\|^2 > 1 - \frac{\varepsilon}{2\Delta(G)}$. Using this estimate, the fact that $\langle Lp, q\rangle = \langle Lq, p\rangle = 0$, and (43) we get

$$\begin{aligned} \langle L_1 f, f\rangle &\geq \langle Lf, f\rangle = \langle Lp, p\rangle + \langle Lq, q\rangle \\ &\geq (l - \frac{\varepsilon}{2})\|q\|^2 > (l - \frac{\varepsilon}{2})(1 - \frac{\varepsilon}{2\Delta(G)}) \geq l - \varepsilon \ . \end{aligned}$$

The other possibility to consider is the case when $\|g\|^2 > \delta = \frac{\varepsilon}{8n\Delta(G)}$. In this case let $B := L_1 - L(G)$ and let $F := E(G_1) \setminus E(G)$. If $h = p+q$ where $p = \sum_{i=1}^n \alpha_i f^{(i)} \in N$, $q \perp N$, then we see as in (51) that

$$|\alpha_i| = |\langle h, f^{(i)}\rangle| < \sqrt{\delta}\|h\|$$

and hence $\|p\|^2 < n\delta\|h\|^2$, so $\|q\|^2 > (1 - n\delta)\|h\|^2$. Therefore

$$\langle L_1 h, h\rangle \geq \langle Lh, h\rangle = \langle Lp, p\rangle + \langle Lq, q\rangle \geq (l - \frac{\varepsilon}{2})\|q\|^2 > (l - \varepsilon)\|h\|^2 \ . \tag{52}$$

Finally:

$$\begin{aligned}
\langle L_1 f, f\rangle &= \langle L_1 g, g\rangle + 2\langle L_1 g, h\rangle + \langle L_1 h, h\rangle \\
&\geq (l-\varepsilon)\|h\|^2 + \langle Bg, g\rangle + 2\langle L_1 g, h\rangle \\
&= (l-\varepsilon)\|h\|^2 + \sum_{uv\in F} (g_u - g_v)^2 + 2 \sum_{uv\in E(G_1)} (g_u - g_v)(h_u - h_v) \\
&\geq (l-\varepsilon)\|h\|^2 + m\sum_{u\in U} g_u^2 - 2 \sum_{uv\in E(G_1)} g_u h_v \\
&\geq (l-\varepsilon)\|f\|^2 + (m-l)\|g\|^2 - 2\sum_{uv\in F_1} g_u h_v
\end{aligned}$$

where $F_1 = F \cup E(U, \bar{U}) \subseteq E(G_1)$, and it is assumed that $u \in U, v \notin U$. It remains to show that

$$(m-l)\|g\|^2 - 2\sum_{uv\in F_1} g_u h_v \geq 0\,. \tag{53}$$

By the Cauchy-Schwartz inequality and assuming that each edge $uv \in F_1$, $u \in U$, has different endvertex $v \notin U$, we estimate:

$$\Big(\sum_{uv\in F_1} g_u h_v\Big)^2 \leq \sum_{uv\in F_1} |g_u|^2 \sum_{uv\in F_1} |h_v|^2 \leq (m + \Delta(G))\|g\|^2 \cdot (\Delta(G)+1)\|h\|^2 \quad .$$

This inequality and the assumption $\|g\|^2 > \delta$ imply that

$$(m-l)\|g\|^2 - 2\sum_{uv\in F_1} g_u h_v \geq (m-l)\sqrt{\delta} - 2\sqrt{m+\Delta(G)}\sqrt{\Delta(G)+1}\sqrt{1-\delta}\,.$$

Obviously, the last expression is ≥ 0 if m is large enough. It should be added that m depends on l, $\Delta(G)$ and $\delta = \delta(\varepsilon, n, \Delta(G))$ but not on f. This finally establishes (53). Thus we succeeded to show $\langle L_1 f, f\rangle \geq l - \varepsilon$, and consequently that $\lambda_1(G_1) \geq l - \varepsilon$.

It is clear that adding edges to a graph cannot decrease the isoperimetric number. Therefore there exists a graph G_2 which can be obtained from G_1 by adding finitely many edges so that $i(G_2) \geq i'(G) - \varepsilon$. Clearly, also $\lambda_1(G_2) \geq \lambda_1(G_1) \geq l - \varepsilon$.

Let $S \subset V(G_2)$ be the set containing all vertices of degree greater than $\Delta'(G)$ and all their neighbors. Let G_3 be the graph obtained from G_2 by adding m parallel edges between any two vertices of S, where $m = \Delta'(G)|S|$.

Choose a finite $U_1 \subset V(G_3)$ such that $e_{G_3}(U_1, \bar{U}_1)/|U_1| \leq i(G_3) + \varepsilon$ (the index G_3 in $e_{G_3}(U_1, \bar{U}_1)$ represents that the edges are in the graph G_3). If $U_1 \cap S = \emptyset$, then let $U := U_1$, otherwise let $U := U_1 \cup S$. So U either contains S, or it is disjoint from S. Therefore no vertex adjacent to U in G_2 has degree greater than $\Delta'(G)$. It is easily seen that in each case

$$\frac{e_{G_2}(U, \bar{U})}{|U|} = \frac{e_{G_3}(U, \bar{U})}{|U|} \leq \frac{e_{G_3}(U_1, \bar{U}_1)}{|U_1|} \leq i(G_3) + \varepsilon \leq i'(G) + \varepsilon \tag{54}$$

since $m = \Delta'(G)|S|$.

Now we may repeat the first part of the proof for the graph G_3, using $\Delta'(G)$ instead of Δ. Note that in (48) we need the fact that $n_v \leq \Delta'(G)$ for each vertex v adjacent to

U. This completes the proof since $i(G_3)$ and $\lambda(G_3)$ are arbitrarily close to their essential values. □

Cheeger inequality of Theorem 3.10 extends to infinite graphs as shown by the next theorem [Mo4].

THEOREM 6.9 *For an arbitrary locally finite graph G with bounded degrees*

$$i(G) \le \sqrt{\lambda_1(G)(2\Delta(G) - \lambda_1(G))} \tag{55}$$

and

$$i'(G) \le \sqrt{\lambda_1'(G)(2\Delta'(G) - \lambda_1'(G))}\ . \tag{56}$$

PROOF. The spectrum $\sigma_L(G)$ is closed, so $\lambda_1 = \lambda_1(G) \in \sigma_L(G)$. For each small enough $\varepsilon > 0$ there is a function $f \in \ell^2(V(G))$ with finite support (only finitely many f_v are nonzero) and with $\|f\| = 1$ such that

$$\langle Lf, f\rangle \le \lambda_1 + \varepsilon \le \Delta(G)\ . \tag{57}$$

If

$$\eta := \sum_{uv\in E(G)} |f_u^2 - f_v^2|$$

then it can be shown by the summation *per partes* that

$$\eta \ge i(G) \tag{58}$$

(see the proof of Theorem 3.10). On the other hand,

$$\begin{aligned}
\eta^2 &= \Big(\sum_{uv\in E} |f_u^2 - f_v^2|\Big)^2 = \Big(\sum_{uv\in E} |f_u + f_v||f_u - f_v|\Big)^2 \\
&\le \sum_{uv\in E} (f_u + f_v)^2 \cdot \sum_{uv\in E} (f_u - f_v)^2 \\
&= \sum_{uv\in E} (2f_u^2 + 2f_v^2 - (f_u - f_v)^2) \cdot \langle Lf, f\rangle \\
&= \Big(2\sum_{v\in V} \mathrm{d}_v f_v^2 - \langle Lf, f\rangle\Big) \cdot \langle Lf, f\rangle \\
&\le (2\Delta(G)\|f\|^2 - \langle Lf, f\rangle)\langle Lf, f\rangle \\
&\le 2\Delta(G)(\lambda_1 + \varepsilon) - (\lambda_1 + \varepsilon)^2\ .
\end{aligned} \tag{59}$$

In the first inequality we used the Cauchy-Schwartz inequality, while in the last one we needed (57). Since ε was arbitrarily small, it follows that $i^2(G) \le \eta^2 \le 2\Delta(G)\lambda_1 - \lambda_1^2$ and the proof of (55) is done.

To prove (56), let G_1 be a graph obtained from G by adding finitely many edges and such that $i(G_1) \ge i'(G) - \varepsilon$ where $\varepsilon > 0$ is arbitrarily small again. As we know from the proof of Theorem 6.8, there is a graph G_2 obtainable from G_1 by addition of finitely many edges such that $\lambda_1(G_2) \ge \lambda_1'(G) - \varepsilon$. Since $i(G_2) \ge i(G_1)$, we have $i(G_2) \ge i'(G) - \varepsilon$.

Let S be the set of vertices of G_2 having degree $> \Delta'(G)$. The set S is clearly finite. Since $\lambda_1' = \lambda_1'(G) = \lambda_1'(G_2)$ is in the essential spectrum, there are arbitrarily many unit

functions $f^{(i)}$, $i = 1, 2, ...$ such that $\langle L(G_2)f^{(i)}, f^{(i)}\rangle \leq \lambda_1' + \varepsilon$, and such that $\langle f^{(i)}, f^{(j)}\rangle = 0$ for $i \neq j$. Let us take $N = |S| + 1$ such functions $f^{(i)}$. They are linearly independent, so any nontrivial linear combination is nonzero. On the other hand, there exist $\alpha_1, \alpha_2, \ldots, \alpha_N$ with some $\alpha_i \neq 0$ such that $\sum_{i=1}^N \alpha_i f^{(i)} =: f$ has the values $f_v = 0$ for each $v \in S$. If we require that $\sum \alpha_i^2 = 1$, then

$$\|f\|^2 = \langle \sum_{i=1}^N \alpha_i f^{(i)}, \sum_{i=1}^N \alpha_i f^{(i)} \rangle = \sum_{i=1}^N \alpha_i^2 = 1 \ .$$

The functions $f^{(i)}$ may also be assumed to satisfy $\|L(G_2)f^{(i)} - \lambda_1' f^{(i)}\| \leq \varepsilon/N$. Then:

$$\begin{aligned}
\langle L(G_2)f, f\rangle &= \sum_{i=1}^N \sum_{j=1}^N \alpha_i \alpha_j \langle L(G_2)f^{(i)}, f^{(j)}\rangle \\
&= \sum_{i=1}^N \alpha_i^2 \langle \lambda_1' f^{(i)}, f^{(i)}\rangle + \sum_{i=1}^N \sum_{j=1}^N \alpha_i \alpha_j \langle L(G_2)f^{(i)} - \lambda_1' f^{(i)}, f^{(j)}\rangle \\
&\leq \lambda_1' + \sum_{i=1}^N \sum_{j=1}^N |\alpha_i \alpha_j| \|L(G_2)f^{(i)} - \lambda_1' f^{(i)}\| \cdot \|f^{(j)}\| \\
&\leq \lambda_1' + \frac{\varepsilon}{N} \sum_{i=1}^N \sum_{j=1}^N |\alpha_i \alpha_j| \leq \lambda_1' + \varepsilon.
\end{aligned}$$

Now we may carry out the same calculation as to obtain (58) and (59), this time for G_2. The inequality $\mathrm{d}_v f_v^2 \leq \Delta'(G) f_v^2$ is clearly satisfied, and the only remaining fact to verify is $\lambda_1' + \varepsilon \leq \Delta'(G)$. But we have shown this by (43) for any graph with $\delta'(G) \geq 1$. The remaining case $\delta'(G) = 0$ is unimportant since in this case $i'(G) = 0$ and $l = 0$, so (56) is trivial. □

6.3 Amenability

In this section we shall shortly exhibit the notion of amenability of infinite graphs. This concept was originally introduced as a property of locally compact groups. We refer to [Pa, Pi] for more information.

Let Γ be a locally compact group. By $L^\infty(\Gamma)$ we denote the set of all functions $\Gamma \to \mathbf{R}$ which are bounded a.e. with respect to the Haar measure $\lambda(.)$ on Γ. The group Γ is *amenable* if $L^\infty(\Gamma)$ has an *invariant mean*, i.e., a linear functional $m : L^\infty(\Gamma) \to \mathbf{R}$ which satisfies the following conditions:

(i) For $f \in L^\infty(\Gamma)$, if $f \geq 0$ (a.e.) then $m(f) \geq 0$.

(ii) $m(\chi_\Gamma) = 1$, where χ_Γ is the constant function 1 on Γ.

(iii) It is Γ-invariant, i.e., $m(g \cdot f) = m(f)$ for every $g \in \Gamma$. (Note that $(g \cdot f)(x) = f(g^{-1}x)$.)

By a theorem of Følner [Fo], the amenability is equivalent to the following condition:

(F) Given $\varepsilon > 0$ and a compact set $K \subseteq \Gamma$ there is a Borel set $U \subseteq \Gamma$ of positive finite measure $\lambda(U) < \infty$ such that

$$\lambda(kU \Delta U) < \varepsilon \lambda(U)$$

for all $k \in K$, where Δ denotes the symmetric difference of sets.

For a discrete group, the Haar measure counts the number of elements of the set. Then it is easy to see that (F) is equivalent to:

(F') For every $\varepsilon > 0$ and finite $K \subseteq \Gamma$ one can find a finite set $U \subseteq \Gamma$ such that

$$|KU \Delta U| < \varepsilon |U| \ .$$

LEMMA 6.10 *Let Γ be a group generated by a finite set of generators $S = \{g_1, \ldots, g_k\}$. Then Γ is amenable if and only if for every $\varepsilon > 0$ there is a finite set $U \subseteq \Gamma$ such that $|SU \setminus U| < \varepsilon |U|$.*

PROOF. ($\Rightarrow$) Let $K := S \cup \{e\}$, where e is the identity in Γ. Then $KU \Delta U = SU \setminus U$. We are done by the amenability of Γ.

($\Leftarrow$) Choose $\varepsilon > 0$ and a finite $K \subseteq \Gamma$, $K = \{k_1, k_2, \ldots, k_t\}$. It may be assumed that $e \notin K$. If k_i can be written as a word of length $l(i)$ in terms of $S \cup S^{-1}$, let

$$\varepsilon_i := \frac{\varepsilon}{2t \cdot l(i)}$$

and let $U \subseteq \Gamma$ be a set for which $|SU \setminus U| < \varepsilon' |U|$, where $\varepsilon' = \min \varepsilon_i$. For each generator $g_j \in S$, $|g_j U \setminus U| \leq |SU \setminus U| < \varepsilon' |U|$. From this we also see that $|g_j U \cap U| > (1 - \varepsilon')|U|$, therefore also $|g_j^{-1} U \cap U| > (1 - \varepsilon')|U|$, so $|g_j^{-1} U \setminus U| < \varepsilon' |U|$. It follows that $|k_i U \setminus U| < l(i)\varepsilon' |U| \leq \frac{\varepsilon}{2t} |U|$. This implies that $|KU \setminus U| < \frac{\varepsilon}{2} |U|$. Since $|KU| \geq |U|$, we get $|KU \triangle U| < \varepsilon |U|$. □

COROLLARY 6.11 *A finitely generated infinite group Γ is amenable if and only if the Cayley graph $\mathrm{Cay}(\Gamma, S)$ with respect to some (and hence every) finite generating set S has the isoperimetric number $i(\mathrm{Cay}(\Gamma, S)) = 0$.*

By Corollary 6.11 it follows trivially that every finitely generated group with polynomial or subexponential growth is amenable. The converse is not true. For example, all soluble groups are amenable but some of them have exponential growth [Ro].

The importance of Corollary 6.11 lies in the fact that it gives a possibility to extend the notion of amenability to graphs in such a way that a finitely generated group Γ is amenable if and only if it has an amenable Cayley graph. So, let us call a graph G *amenable* if $i(G) = 0$.

The case of graphs with bounded degrees was investigated in detail by Peter Gerl and we refer to his works [Ge1, Ge2] where several conditions equivalent to amenability are derived. For a possibility of extending the notion to graphs with unbounded degrees see [Mo4]. We refer to [S-W] for additional results on amenability of graphs.

6.4 Random walks on infinite graphs

The *transition matrix* $P(G) = [p_{uv}]$ of a locally finite infinite graph G has entries $p_{uv} = a_{uv}/\mathrm{d}_u$. This matrix is usually assumed to act on the Hilbert space $\ell^2_d(V)$ endowed with the inner product is given by

$$\langle f, g\rangle_d = \sum_{v\in V} f_v g_v \mathrm{d}_v$$

and whose elements f satisfy $\langle f, g\rangle_d < \infty$. Then $P(G)$ defines a bounded self-adjoint linear operator on $\ell^2_d(V)$ (even though the matrix $P(G)$ need not be symmetric). It is important that G is locally finite but the requirement $\Delta(G) < \infty$ is not needed for $P(G)$ to be everywhere defined and bounded. The spectrum $\sigma_P(G)$ of $P(G)$ is real and always contained in the interval $[-1, 1]$ (cf., e.g., [M-W]). We define

$$\rho_1(G) := \sup \sigma_P(G).$$

The Rayleigh characterization of ρ_1 similar to (42) is

$$\rho_1(G) = \sup \left\{ \frac{\langle P(G)f, f\rangle_d}{\langle f, f\rangle_d} \;\Big|\; f \in \ell^2_d(V), f \neq 0 \right\}. \tag{60}$$

We can also define the essential spectrum and set $\rho'_1(G)$ to be the supremum of the essential spectrum of $P(G)$.

Relations between $\rho_1(G), \rho'_1(G)$ and isoperimetric invariants are proved in [Mo4]. They seem to be more natural than the corresponding relations with the Laplacians.

The transition matrix is related to simple random walks on the graph G. The most important problem is the *type problem* for the simple random walks on graphs which asks if the random walk is recurrent or transient. It is well known that the random walk on $\mathbf{Z}^2$ (the 2-dimensional integer lattice) is recurrent, while the random walk on $\mathbf{Z}^3$ is transient. For this type of graphs, the threshold between recurrence and transience lies somewhere between the quadratic and cubic growth (cf. [D-S]). More generally, Varopoulos [Var] proved:

THEOREM 6.12 *The simple random walk on a Cayley graph of a finitely generated group is recurrent if and only if the graph has polynomial growth of degree at most two.*

This result was extended to general (locally finite) infinite graphs by Thomassen [Th] as follows. We say that G satisfies the *connected ϕ-isoperimetric inequality* at the vertex $v_0 \in V(G)$, where $\phi : \mathbf{N} \to \mathbf{N}$, if there is a constant $c > 0$ such that every finite connected subgraph H of G with $v_0 \in V(H)$ satisfies

$$e(V(H), V(G)\backslash V(H)) \geq c\,\phi(|V(H)|).$$

Let us observe that G satisfies the connected isoperimetric inequality for the identity function if and only if $i(G) > 0$.

THEOREM 6.13 *If G satisfies the connected ϕ-isoperimetric inequality at some vertex v_0 and if $\sum_{k=1}^{\infty} \phi(k)^{-2} < \infty$, then the simple random walk on G is transient.*

For further reading we refer to [Woe].

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