Eigenvalues in Combinatorial Optimization *

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Abstract

In the last decade many important applications of eigenvalues and eigenvectors of graphs in combinatorial optimization were discovered. The number and importance of these results is so fascinating that it makes sense to present this survey.

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Contents

1 Introduction

The application of eigenvalue methods in combinatorial optimization has already a long history. The first eigenvalue bounds on the chromatic number were formulated by H. S. Wilf and A. J. Hoffman already at the end of sixties. Historically, the next applications, due to M. Fiedler and Donath and Hoffman in 1973, concerned the area of graph partition. A very important use of eigenvalues is the Lovász's notion of the theta-function from 1979. Using it, he solved the long standing Shannon capacity problem of the 5-cycle. Moreover, the theta-function provides the only known way to compute the chromatic number of perfect graphs in polynomial time.

Next strong result was the use of eigenvalues in the construction of supercontrators and expanders by Alon and Milman 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 analysed the behaviour of the theta-function on random graphs, and introduced the eigenvalues in the clustering. Isoperimetric properties of graphs have also a crucial role in designing random polynomial time algorithm for approximating volume of convex bodies (cf., e.g., [87]).

Recently, 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 used the eigenvalue approach in the study of the quadratic assignment problem and general graph partition problems, Delorme and Poljak in the max-cut problem, and Juvan and Mohar in the labelling problems.

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 edge-connectivity, separation properties, bandwidth and cutwidth, and bounds on the chromatic number and stable sets in Sections 4.1, 4.2, and 4.3. 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. It seems that the finest estimates can be obtained in this way, in particular for the partition problems.

Different 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.

The common point of the most important among the presented applications is the possibility of the change to a "continuous optimization". In such cases there is a possibility of introducing a parameter $u \in \boldsymbol{R}^n$ and optimizing when U is restricted to be an element of a convex set $K \subseteq \boldsymbol{R}^n$. This way we get improved bounds or methods for the problems in question. A classical example is the Lovász' ϑ-function. 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 (Theorems 2.1 and 2.3, Corollary 2.4), partition (Theorem 2.18, Corollaries 2.19 and 2.20), max-cut (Lemma 2.10), stable sets and coloring (Theorems 4.11 and 4.15), bandwidth (Theorem 3.1 and the inequality (44)), etc.

Our survey is organized according to the types of the combinatorial optimization problems: partition, ordering, coloring and stable sets, routing. We also include a short section on the isometric embedding; especially because the bounds there rely on another property of eigenvalues, the Sylvester's inertia law. Appendix A contains some information about the computational aspects, and Appendix B collects known results on eigenvalues of random matrices. Some basic properties of eigenvalues are recalled in the following subsection.

There are several existing books and survey papers concerning graph eigenvalues, e.g., [16, 34, 33, 47, 96, 98]. We do not intend to overlap our presentation with their contents. Therefore we restrict ourselves to some problems which can be classified as applications in combinatorial optimization, and that are not treated in any of the works mentioned above. In particular, we do not include discussion on expander graphs (which are accessible only via eigenvalue methods) and their applications, although they are quite important tool in the design of algorithms and several other areas of theoretical computer science.

The present text is biased by the viewpoint and the interests of the authors and can not be complete. Therefore we apologize to all those who feel that their work is missing in the references or has not been emphasized sufficiently in the text.

We thank Ch. Delorme, F. Rendl and M. Laurent, with whom we discussed parts of the topic presented here, and who also provided us with several references.

1.1 Matrices and eigenvalues of graphs

Graphs are assumed to be finite and undirected (unless stated otherwise), multiple edges and loops are permitted. It is in the nature of some problems that only simple graphs make sense, e.g., when speaking about stable sets or colorings (cf. Section 4). In such cases graphs will be assumed to be simple. In some other cases, we will allow more general objects – *weighted graphs*, i.e., each edge $uv \in E(G)$ has a real weight $w(uv) > 0$. (We also set $w(uv) := 0$ if u and v are not adjacent.) Unweighted graphs are special case of weighted ones if we define $w(uv)$ as the number of edges between v and u. If G is a graph of order n, the *adjacency matrix* $A(G) = [a_{uv}]$ of G is an $n \times n$ matrix with rows and columns indexed by $V(G)$ and entries a_{uv} $(u, v \in V(G))$ equal to the number of edges between vertices u and v. Consistent with this is the definition of the adjacency matrix of a weighted graph with weights $w(uv)$ where $a_{uv} = w(uv)$. The *degree* $deg(v)$ of a vertex $v \in V(G)$ is equal to the number of edges adjacent to v. In the weihgted case we define the degree of v as the sum of weights of edges adjacent to v. Denote by $D(G)$ the diagonal matrix indexed by $V(G)$ and with vertex degrees on the diagonal, i.e., $d_{vv} = deg(v),\ v \in V(G)$, and $d_{uv} = 0$ if $u \neq v$. The difference

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

is called the (*difference*) *Laplacian matrix* of G. It is easy to see that for a vector $x \in \ell^2(V(G))$ (a vector of dimension $|V(G)|$ with coordinates x_v, $v \in V(G)$, corresponding to vertices of G) we have

$$x^T L(G)x = \sum_{u,v} a_{uv}(x_u - x_v)^2 \tag{2}$$

which in case of a simple graph G reduces to

$$x^T L(G)x = \sum_{uv \in E(G)} (x_u - x_v)^2 . \tag{3}$$

The matrix $L(G)$ is real symmetric, so it has $n = |V(G)|$ real eigenvalues $\lambda_1 \leq \lambda_2 \leq \ldots \leq \lambda_n$ (repeated according to their multiplicities). By (2) it is immediate that $L(G)$ is positive semidefinite. It also follows easily from (2) that $\lambda_1 = 0$ with a corresponding eigenvector $\mathbf{1} = (1, 1, \ldots, 1)^T$, and that $\lambda_2 > 0$ if and only if the graph is connected (see Section 2.2). We will use the notation $\lambda_k(G)$ to denote the k-th smallest eigenvalue of $L(G)$ (respecting the multiplicities), and generally, if M is a matrix with real eigenvalues, we

denote by $\lambda_k(M)$ the k-th smallest eigenvalue of M. To denote the maximal eigenvalue of M we use the symbol $\lambda_{\max}(M)$. Consistently with this notation we will sometimes use $\lambda_{\min}(M)$ instead of $\lambda_1(M)$.

There are several useful min-max formulas for the expression of eigenvalues of a symmetric matrix and their sums. If M is a real symmetric matrix of order $n \times n$ then

$$\begin{aligned} \lambda_1(M) &= \min\Big\{\frac{x^T M x}{\|x\|^2} \mid 0 \neq x \in \boldsymbol{R}^n\Big\} \\ &= \min\{x^T M x \mid x \in \boldsymbol{R}^n,\ \|x\| = 1\} \end{aligned} \tag{4}$$

and similarly

$$\lambda_{\max}(M) = \max\{x^T M x \mid x \in \boldsymbol{R}^n,\ \|x\| = 1\}. \tag{5}$$

The Rayleigh's characterization (4) has a generalization, the min-max characterization of $\lambda_k(M)$, known also as the Courant-Fisher's expression:

$$\lambda_k(M) = \min_U \max_x \{x^T M x \mid \|x\| = 1,\ x \in U\} \tag{6}$$

where the first minimum is over all k-dimensional subspaces U of $\boldsymbol{R}^n$. Another way of expressing (6) is

$$\lambda_k(M) = \min\{x^T M x \mid \|x\| = 1, x \perp x_i, 1 \leq i < k\} \tag{7}$$

where $x_1, \ldots, x_{k-1}$ are pairwise orthogonal eigenvectors of $\lambda_1, \ldots, \lambda_{k-1}$, respectively. We will also need a result known as Fan's Theorem [44] on the sum of the k smallest eigenvalues of M:

$$\sum_{i=1}^{k} \lambda_i(M) = \min_{x_1,\ldots,x_k} \Big\{\sum_{i=1}^{k} x_i^T M x_i \mid \|x_i\| = 1,\ x_i \perp x_j, 1 \leq i, j \leq k, i \neq j\Big\} \tag{8}$$

where the minimum runs over all pairwise orthogonal k-tuples of unit vectors $x_1, x_2, \ldots, x_k$.

The proofs of the Rayleigh's principle and the Courant-Fisher theorem can be found in standard books on matrix theory, e.g. [83]. A short proof of the Fan's theorem is given in [106].

If G is a (weighted) graph and $L = L(G)$ its Laplacian matrix then by (7)

$$\lambda_2(G) = \min\{x^T L x \mid \|x\| = 1,\ x \perp \mathbf{1}\} \tag{9}$$

since $\mathbf{1}$ is an eigenvector of $\lambda_1(G)$. Fiedler [46] used (9) to get a more useful expression for $\lambda_2(G)$:

$$\lambda_2(G) = 2n \cdot \min \left\{ \frac{\sum_{uv \in E} a_{uv}(x_u - x_v)^2}{\sum_{u \in V} \sum_{v \in V} (x_u - x_v)^2} \mid x \neq c \cdot \mathbf{1} \text{ for } c \in \boldsymbol{R} \right\} \quad (10)$$

where $V = V(G)$, $E = E(G)$, and $n = |V|$. The expression (10) implies a similar expression for $\lambda_{\max}(G)$

$$\lambda_{\max}(G) = 2n \cdot \max \left\{ \frac{\sum_{uv \in E} a_{uv}(x_u - x_v)^2}{\sum_{u \in V} \sum_{v \in V} (x_u - x_v)^2} \mid x \neq c \cdot \mathbf{1} \text{ for } c \in \boldsymbol{R} \right\} . \quad (11)$$

2 Partition Problems

The common question in the partition problems surveyed in this section is to find a partition of the vertex set of a graph into two parts S and $V \setminus S$ such that the edge cut

$$\delta S = \{e = uv \in E(G) \mid u \in S, v \notin S\}$$

satisfies some specific extremal property. This property differs for graph bisection, edge connectivity, isoperimetric property, max-cut problem and clustering. It ranges from maximizing or minimizing $|\delta S|$ to optimization of functions that may depend both on δS and the partition $(S, V \setminus S)$.

It makes sense to introduce another notation which can also be used instead of δS. If A, B are disjoint subsets of $V(G)$ then we denote by $E(A, B)$ the set of edges with one end in A and the other end in B. We also write

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

where w is the edge-weight function of the graph. Clearly, $e(A, B) = |E(A, B)|$ if G is unweighted.

The common initial point for the considered partition problems is to represent a partition $(S, V \setminus S)$ by a ± 1-vector $x_S = (x_{S,i}$ where $x_{S,i} = 1$ for $i \in S$ and $x_{S,i} = -1$ for $i \notin S$. If $w = (w_{ij})$ is an edge-weight function, then the weight $w(\delta S)$ of the cut induced by S can be expressed via the Laplacian matrix (cf. (2)) as follows.

$$w(\delta S) := \sum_{i \in S, j \notin S} w_{ij} = \frac{1}{4} \sum_{i,j \in V} w_{ij}(x_{S,i} - x_{S,j})^2 = \frac{1}{4} x_S^T L(G) x_S \, . \quad (12)$$

The last subsection deals with multi-partition problems, which generalize the bisection problem of Subsection 2.1.

2.1 Graph bisection

Let $G = (V, E)$ be a graph with an even number of vertices. The *bisection width* $bw(G)$ is defined as the minimum number of edges whose deletion disconnects G into two parts of the same size, i.e.

$$bw(G) := \min\{w(\delta S) \mid S \subset V, |S| = \frac{1}{2}|V|\}\,.$$

The most applications of the graph bisection problem are in the area of VLSI (see [84]). The problem of determining $bw(G)$ is NP-complete ([53]), and hence approximative algorithms and bounds on $bw(G)$ come into interest.

The first eigenvalue lower bound on $bw(G)$ was formulated by Donath and Hoffman in [42]. Their bound has been later improved by Boppana [18] as follows. Let n be the number of vertices of G, and $u = (u_1, \ldots, u_n)^T$ a vector of length n.

THEOREM 2.1 *([18]) Let G be a graph of order n. Then*

$$bw(G) \geq \frac{n}{4} \max_u \min_x x^T(L(G) + \mathrm{diag}(u))x \tag{13}$$

where the maximum is taken over all vectors $u \in \boldsymbol{R}^n$ satisfying $\sum_{i=1}^n u_i = 0$, and the minimum is over all vectors $x \in \boldsymbol{R}^n$ satisfying $\sum_{i=1}^n x_i = 0$ and $\|x\| = 1$.

PROOF. Let $(S, V \setminus S), |S| = \frac{1}{2}n$, be a partition which realizes the minimum bisection width, i.e. $w(\delta S) = bw(G)$. Let us define a vector $y = (y_i)$ by $y_i = 1$ for $i \in S$, and $y_i = -1$ for $i \notin S$. Further, let u be a vector with $\sum_{i=1}^n u_i = 0$ which realizes the maximum on the right-hand side of (13). Using (12), we get

$$bw(G) = w(\delta S) = \frac{1}{4} y^T L(G) y\,.$$

We also have

$$y^T \mathrm{diag}(u) y = \sum_{i=1}^n u_i y_i^2 = \sum_{i=1}^n u_i = 0$$

since $y_i^2 = 1$ for every i. Hence

$$\frac{1}{4} y^T (L(G) + \mathrm{diag}(u)) y = bw(G).$$

Finally, since $\|y\|^2 = n$ and $\sum_{i=1}^n y_i = 0$, we have

$$\frac{1}{4} y^T (L(G) + \mathrm{diag}(u)) y \geq \min_x \frac{n}{4} x^T (L(G) + \mathrm{diag}(u)) x$$

where the minimum is taken over all $x \in \boldsymbol{R}^n$ with $\|x\| = 1$ and $\sum_{i=1}^n x_i = 0$. This proves the theorem. □

The main result of [18] is that the lower bound given in the above theorem provides the actual value of $bw(G)$ with a high probability in a certain probabilistic model. Let $\mathcal{G}(n, m, b)$ be the set of graphs with n vertices, m edges, and the bisection width $bw(G) = b$.

THEOREM 2.2 *([18]) Suppose that* $b \leq \frac{1}{2}m - \frac{5}{2}\sqrt{mn \log n}$. *Then the lower bound of Theorem 2.1 is exact for a graph* G *from* $\mathcal{G}(n, m, b)$ *with probability at least* $1 - O(\frac{1}{n})$. □

An important fact is that the bound of Theorem 2.1 is efficiently computable – see the Appendix A. It relies on the concavity of the function $f(u)$ given as

$$f(u) = \min_x x^T (L(G) + \mathrm{diag}(u)) x$$

where the minimum is over all x with $\|x\| = 1$ and $\sum_{i=1}^n x_i = 0$.

For computational purposes, it is convenient to express the bound of Theorem 2.1 as the minimum eigenvalue of a certain matrix. Let $Q = (q_1, \ldots q_{n-1})$ be an $n \times (n-1)$ matrix such that the columns q_i are mutually orthogonal unit vectors satisfying $\mathbf{1}^T q_i = 0$, $i = 1, \ldots, n-1$.

COROLLARY 2.3 *([18]) We have*

$$bw(G) \geq \max_u \frac{n}{4} \lambda_{\min}(Q^T (L(G) + \mathrm{diag}(u)) Q) \tag{14}$$

where the maximum runs over all vectors $u \in \boldsymbol{R}^n$ *with* $\sum_{i=1}^n u_i = 0$. □

The bound of Theorem 2.1 improves a previous bound of Donath and Hoffman, which is formulated in the following corollary.

COROLLARY 2.4 *([42]) We have*

$$bw(G) \geq \max_u \frac{n}{4} \left(\lambda_1(Q^T (L(G) + \mathrm{diag}(u)) Q) + \lambda_2(Q^T (L(G) + \mathrm{diag}(u)) Q) \right)$$

where the maximum is taken over all vectors $u \in \boldsymbol{R}^n$ *such that* $\sum u_i = 0$.

PROOF. The proof easily follows by the application of the Rayleigh quotient (6) to λ_1 and λ_2, and using the Fan's theorem (8). □

Let us note that the original proof of Corollary 2.4 was based on the following *Hoffman-Wielandt inequality* proved in [68]. Let M and N be symmetric matrices of size $n \times n$. Then

$$\sum_{i=1}^{n} \lambda_i(M)\lambda_{n-i+1}(N) \leq tr(MN) \leq \sum_{i=1}^{n} \lambda_i(M)\lambda_i(N) \ . \tag{15}$$

Let us remark that the bounds of Corollaries 2.3 and 2.4 coincide when G is a vertex transitive graph, but there exist instances, e.g. the path of length 3, for which the bound of Boppana is strictly greater than that of Donath-Hoffman. Computational experiments with the Boppana's bound are reported in [118]. It appears that the bound provides a very good estimate on the bisection width also in practice. Some computational experiments with the Donath-Hoffman bound were done earlier in [42] and [30].

A probabilistic algorithm for the bisection width using *randomized rounding* was developed in [126]. It has been proved that, for r-regular graphs and every $0 < \varepsilon < 1$, the algorithm constructs a bisection such the number of edges in the cut does not exceed $bw(G)$ by more than $O\Big(\sqrt{n \ln \frac{1}{\varepsilon}}\Big)$. Another approximation algorithm is presented in [57].

2.2 Connectivity and separation

It was quite early when Fiedler [45] observed that the second smallest Laplacian eigenvalue $\lambda_2(G)$ measures the graph connectivity. He calls $\lambda_2(G)$ the *algebraic connectivity* of G. The use of the name is justified by the following results.

THEOREM 2.5 *([45]) Let G be a simple graph of order n different from the complete graph K_n. Denote by $\nu(G)$ and $\mu(G)$ its vertex- and edge-connectivity, respectively. Then*

(a) $\lambda_2(G) \leq \nu(G) \leq \mu(G)$, *and*

(b) $\lambda_2(G) \geq 2\mu(G)(1 - \cos(\pi/n))$.

In particular, G is connected if and only if $\lambda_2(G) > 0$. □

The algebraic connectivity has many properties similar to other measures of connectivity: $\lambda_2(G) \leq \lambda_2(G+e)$, a vertex deletion can reduce λ_2 by at most 1, $\lambda_2(G-v) \geq \lambda_2(G)-1$, if G is a simple graph, etc. The reader is referred to a survey [96] for more details. Many additional properties obtained by M. Fiedler are also surveyed in [47]. Some properties of la_2 with respect to connectivity were found independently also by Anderson and Morley (see [7]).

By the work of Tanner [129] and later by several other authors (cf. [96]) it became clear that λ_2 measures the connectivity in the following sense: How difficult is to split the graph into two large pieces? More precisely, if $\lambda_2(G)$ is large, then any partition of $V(G)$ into classes $X \cup Y$, where X and Y are both large, has many edges between X and Y. Unfortunately, the converse is not true. For example, a highly connected graph together with an isolated vertex will have λ_2 equal to 0. The basic "folklore" result justifying the above statements is the following inequality:

PROPOSITION 2.6 *Let G be a (weighted) graph of order n. For a subset $X \subset V(G)$ let $w(\delta X)$ be the total weight of edges in δX. Then*

$$w(\delta X) \geq \lambda_2(G)\frac{|X|(n-|X|)}{n}\,. \tag{16}$$

PROOF. Let $x \in \ell^2(V)$ be given by $x_v = 1$ if $v \in X$, and $x_v = 0$ otherwise. Then

$$\sum_{u\in V}\sum_{u\in V}(x_u - x_v)^2 = 2|X|(n-|X|)$$

and

$$\sum_{uv\in E} a_{uv}(x_u - x_v)^2 = \sum_{uv\in \delta X} a_{uv} = w(\delta X).$$

By (10) we get the inequality of the proposition. □

In the same way as above we get from (11):

PROPOSITION 2.7 *If G is a (weighted) graph of order n and $X \subset V(G)$ a subset of vertices then*

$$w(\delta X) \leq \lambda_n(G)\frac{|X|(n-|X|)}{n}\,. \tag{17}$$

□

It is an important consequence of (16) and (17) that in a graph which has all non-trivial Laplace eigenvalues in a small interval ($\lambda_2(G)$ and $\lambda_n(G)$ close to each other), all vertex sets X of the same cardinality have approximately the same number of out-going edges $w(\delta X)$. In particular, this is true for random graphs or for random regular graphs (cf. Appendix B). The consequence of this fact is that many algorithms for problems involving some kind of separation behave very well for random graphs. In fact, to get good vertex partition into sets of given size in a graph, one does not need to be very clever – any partition will do a good job.

Related to the connectivity, but less trivial to establish are *separation properties* of graphs. A set $C \subset V(G)$ is said to *separate* vertex sets $A, B \subset V(G)$ if

(a) A, B, and C partition $V(G)$ and

(b) no vertex of A is adjacent to a vertex of B.

In applications one is interested in small sets C separating relatively large sets A and B. Usually we want that $|C| = o(n)$ and $|A| = \Omega(n)$, $|B| = \Omega(n)$. The following results show that graphs G with large $\lambda_2(G)$ do not contain small separators.

THEOREM 2.8 *Let G be a graph and $w : E(G) \to \boldsymbol{R}^+$ an arbitrary non-negative edge-weighting of G. Denote by $\lambda_2 = \lambda_2(G_w)$ the first non-trivial Laplace eigenvalue of the corresponding weighted graph G_w, and by $\Delta = \Delta(G_w)$ the maximal (weighted) degree of G_w. If $C \subset V(G)$ separates vertex sets A, B then*

$$|C| \geq \frac{4\lambda_2|A||B|}{\Delta n - \lambda_2|A \cup B|} \tag{18}$$

and

$$|C| \geq \frac{1}{2\lambda_2}\Big(- n(\Delta - \lambda_2) + \sqrt{n^2(\Delta - \lambda_2)^2 + 16\lambda_2^2|A||B|}\Big) \ . \tag{19}$$

PROOF. Let $x \in \ell^2(V(G))$ be defined by $x_v = -1$ if $v \in A$, $x_v = 1$ if $v \in B$, and $x_v = 0$ if $v \in C$. By (10) we have:

$$\lambda_2 \leq 2n\frac{e(A,C) + e(B,C)}{8|A||B| + 2|C||A \cup B|} \leq \frac{n\Delta|C|}{4|A||B| + |C||A \cup B|} \ . \tag{20}$$

By rearranging (20) we get (18). If we use in (18) the relation $|A \cup B| = n - |C|$ we get a quadratic inequality for $|C|$ which yields (19). □

A slightly weaker version of (18) was obtained by Alon and Milman [6, Lemma 2.1].

Of course, using (18) or (19) makes sense only in case when $|A \cup B| \geq n/2$. Otherwise we should use in (20) the inequality $e(A,C)+e(B,C) \leq \Delta|A \cup B|$ instead of $e(A,C) + e(B,C) \leq \Delta|C|$ which was used above.

Theorem 2.8 implies that graphs containing small separators separating two large sets (e.g. graphs of bounded genus) have small λ_2. In other words, when λ_2 is large we see that any separator C separating large sets contains many vertices. For example, random graphs (edge probability $\frac{1}{2}$, cf. Appendix B) have $\lambda_2 = \frac{n}{2} - O(\sqrt{n \log n})$ and $\Delta = \frac{n}{2} + O(\sqrt{n \log n})$. If we want a separator C separating sets of sizes $c_1 n + o(n)$ and $c_2 n + o(n)$, respectively, we get from (19)

$$|C| \geq 4n\sqrt{c_1 c_2} + o(n) \ .$$

Concerning separation properties related to eigenvalues we also refer to [114].

2.3 Isoperimetric numbers

In [6] some inequalities of the isoperimetric nature relating λ_2 and some other quantities in graphs are presented. These results have analytic analogues [61] in the theory of Riemannian manifolds where the role of λ_2 is played by the smallest positive eigenvalue of the Laplacian differential operator on the Riemannian manifold. Approximately at the same time Buser [24] and Dodziuk [41] also discovered isoperimetric inequalities involving the Laplace eigenvalues of graphs.

In [5] expanders and graphs with large λ_2 are related. Expanders can be constructed from graphs which are called *c-magnifiers* ($c \in \boldsymbol{R}^+$). These are graphs which are highly connected according to the following property. For every set X of vertices of G with $|X| \leq \frac{n}{2}$, the neighbourhood $N(X)$ of X contains at least $c|X|$ vertices. In [5] it is shown that a graph G is $\frac{2\lambda_2}{\Delta+2\lambda_2}$-magnifier and, conversely, if G is a c-magnifier then $\lambda_2(G) \geq \frac{c^2}{4+2c^2}$. The first result is based on Proposition 2.6, while the second one is a discrete version of the Cheeger's inequality [25] from the theory of Riemannian manifolds.

A strong improvement over the Alon's discrete version of the Cheeger's inequality was obtained by Mohar [95] in connection with another problem. The *isoperimetric number* $i(G)$ of a graph G is equal to

$$i(G) = \min\Big\{\frac{|\delta X|}{|X|} \mid X \subset V, 0 < |X| \leq \frac{|V|}{2}\Big\}.$$

This graph invariant is NP-hard to compute, and even obtaining any lower bounds on $i(G)$ seems to be a difficult problem. The following easy derived bound

$$i(G) \geq \frac{\lambda_2(G)}{2} \tag{21}$$

is so important that it initiated a great interest in the study of eigenvalues of graphs. All started with an application of (21) in the construction of expander graphs (cf. [5, 89, 90, 15, 88]) and this motivated much of the research surveyed in this paper. (Slightly before the interest in the Laplacian of graphs was influenced by its use in the analysis of the Laplace differential operator on Riemannian manifolds, cf. [22, 24, 41]).

The inequality (21) holds also for weighted graphs by the obvious change in the definition of $i(G)$. It follows easily from Proposition 2.6. It is notably important that there is also an upper bound on $i(G)$ in terms of $\lambda_2(G)$. One of the strongest such inequalities is the following [95]:

THEOREM 2.9 *([95]) Let G be a simple graph on at least 3 vertices. Then*

$$i(G) \leq \sqrt{\lambda_2(2\Delta - \lambda_2)} \tag{22}$$

where Δ is the maximal vertex degree in G, and $\lambda_2 = \lambda_2(G)$. □

Theorem 2.9 is a discrete version of Cheeger's inequality [25] relating the first non-trivial eigenvalue of the Laplace differential operator on a compact Riemannian manifold to an isoperimetric constant of the manifold. Discrete versions of the Cheeger's bound were found by Alon [5] (vertex version as mentioned above), Dodziuk [41] (for infinite graphs), Varopoulos [130] (also for the infinite case), Mohar [94, 95], Sinclair and Jerrum [124] (in terms of Markov chains), Friedland [49]. Cf. also Diaconis and Stroock [39].

There are other definitions of isoperimetric constants of graphs. For example, define for $X \subseteq V(G)$

$$S(X) = \sum_{v \in X} \deg(v) \ .$$

Then one can define the following version of the isoperimetric number:

$$i'(G) = \min\Big\{\frac{|\delta X|}{S(X)} \mid X \subset V, 0 < S(X) \leq |E(G)|\Big\}.$$

(Note that $|E(G)| = \frac{1}{2}S(V(G))$.) Similar eigenvalue bounds as (21) and (22) can be derived for $i'(G)$:

$$i'(G) \geq \frac{1 - \lambda_{\max}(P)}{2} \tag{23}$$

where $P = [p_{uv}]$ is the transition matrix of the random walk on G, i.e., $p_{uv} = a_{uv}/\deg(u)$, and a_{uv} is the element of the adjacency matrix of G. The reader is referred to [94] for details. There is also the corresponding upper bound of Cheeger's type, derived for infinite graphs by Mohar [94], and for finite graphs by Sinclair and Jerrum [124]. Cf. also [39].

A similar isoperimetric quantity as $i'(G)$ was introduced by Friedland [49] who defines for $U \subset V(G)$, $U \neq \emptyset$,

$$\epsilon(U) = \min_{\emptyset \neq V \subseteq U} \frac{|\delta V|}{S(V)}$$

and shows that the smallest eigenvalue $\lambda_1(L_U)$ of the principal submatrix of $L(G)$ whose rows and columns are indexed by U is bounded by

$$\lambda_1(L_U) \geq \min_{v \in U} \frac{\deg(v)}{2} \epsilon(U)^2 \ . \tag{24}$$

Friedland [49] also provides several norm estimates for $\lambda_1(L_U)$.

There are vertex oriented isoperimetric inequalities for graphs using eigenvalues which are appropriate for some other purposes, e.g., [5, 87]. Lovász and Simonovits [87], and Dyer, Frieze and Kannan [43] used the isoperimetric number in a random polynomial time algorithm for estimating the volume of a convex body.

2.4 The maximum cut problem

A weighted graph G with an edge-weight function w will be denoted as a pair (G, w) in this subsection (which differs from our standard notation), because we need to consider some operations with the weight functions.

The *maximum cut* problem, or shortly the *max-cut* problem, is to find a subset $S \subset V$ for which the weight $w(\delta S) := \sum_{e \in \delta S} w(e)$ is maximum. Let $mc(G, w)$ denote the value of the maximum cut. An eigenvalue upper bound

$$mc(G, w) \leq \frac{n}{4} \lambda_{\max} L(G, w) \tag{25}$$

was first studied by Mohar and Poljak in [99]. Later, an optimized eigenvalue bound has been introduced by Delorme and Poljak in [35]:

$$mc(G,w) \leq \min_u \frac{n}{4}\lambda_{\max}(L(G,w) + \mathrm{diag}(u)) =: \varphi(G,w) \tag{26}$$

where the minimum is taken over all $u \in \boldsymbol{R}^n$ such that $\sum u_i = 0$. The validity of (26) is based on the following lemma.

LEMMA 2.10 *We have*

$$mc(G,w) \leq \frac{n}{4}\lambda_{\max}(L(G,w) + \mathrm{diag}(u)) \tag{27}$$

for every vector $u \in \boldsymbol{R}^n$ *satisfying* $\sum u_i = 0$.

PROOF. Let S be a subset of V for which $w(\delta S)$ is maximum. Let us consider a vector $y \in \boldsymbol{R}^n$ defined by $y_i = 1$ for $i \in S$ and $y_i = -1$ for $i \notin S$. Observe that y satisfies $\|y\|^2 = n$, and $\sum_{i=1}^n u_i y_i^2 = 0$ for a vector $u \in \boldsymbol{R}^n$ with $\sum_{i=1}^n u_i = 0$. By (12) we have:

$$\begin{aligned} mc(G,w) &= w(\delta S) = \frac{1}{4}y^T L y \\ &= \frac{1}{4}(y^T L y + \sum_{i=1}^n u_i y_i^2) \\ &\leq \max_{\|x\|^2=n} \frac{1}{4}(x^T L x + x^T \mathrm{diag}(u) x) \\ &= \frac{n}{4}\lambda_{\max}(L + \mathrm{diag}(u)) \ . \end{aligned}$$

□

We call u with $\sum_{i=1}^n u_i = 0$ a *correcting vector*. Observe that the bound of (25) corresponds to the choice of correcting vector $u = 0$. Let $\varphi(G,w)$ denote the minimum in (26). In fact, the minimum is achieved for a unique correcting vector u. The optimum correcting vector u has a dual characterization by Theorem 2.11.

For a linear subspace $\mathcal{E} \subset \boldsymbol{R}^n$, let $\mathcal{C}(\mathcal{E})$ denote the convex cone generated by vectors $(x_1^2, x_2^2, \ldots, x_n^2)^T$ for $x = (x_1, x_2, \ldots, x_n)^T \in \mathcal{E}$.

THEOREM 2.11 *([35]) Let* $\mathcal{E}$ *be the eigenspace of the maximum eigenvalue* λ_{max} *of* $L(G) + \mathrm{diag}(u)$ *for a correcting vector* u. *Then* u *is the optimum correcting vector if and only if* $(1,1,\ldots,1)^T \in \mathcal{C}(\mathcal{E})$. □

The bound $\varphi(G,w)$ has some pleasant properties. It can be computed in polynomial time with an arbitrarily prescribed precision, and it seems to provide a good estimate on $mc(G,w)$. Let $mc(G)$ and $\varphi(G)$ denote the max-cut and the eigenvalue bound for an unweighted graph G. Asymptotically, the ratio $\varphi(G)/mc(G)$ tends to 1 for a random graph G, but the worst case ratio of $\varphi(G,w)/mc(G,w)$ for $w \geq 0$ is not known. (It does not make sense to investigate the ratio with general w, since $mc(G,w)$ may become zero.) So far the worst known case is the 5-cycle C_5, for which the ratio is $\varphi(G)/mc(G) = \frac{25+5\sqrt{5}}{32} = 1.1306\ldots$. It remains open whether $\varphi(G,w)/mc(G,w) \leq 1.131$ for all graphs with non-negative weights. The conjecture was confirmed for planar graphs in [35], and other classes of graphs in [36, 37]. We recall here the result for planar graphs. First we need an auxiliary result about subadditivity of φ with respect to amalgamation which we present without the proof.

Let (G_1,w^1) and (G_2,w^2) be a pair of weighted graphs on vertex sets V_1 and V_2. We define the *amalgam* (G_1+G_2,w) as the weighted graph on $V_1 \cup V_2$ where

$$w_{ij} = \begin{cases} w^1_{ij} & \text{for } ij \in V_1 \\ w^2_{ij} & \text{for } ij \in V_2 \\ w^1_{ij} + w^2_{ij} & \text{for } ij \in V_1 \cap V_2 \\ 0 & \text{elsewhere .} \end{cases}$$

LEMMA 2.12 *([35]) We have $\varphi(G_1+G_2,w) \leq \varphi(G_1,w^1) + \varphi(G_2,w^2)$ for any pair of weighted graphs (G_1,w^1) and (G_2,w^2).* □

THEOREM 2.13 *([35]) Let $G=(V,E)$ be a planar graph with nonnegative edge weight function w. Then*

$$\varphi(G,w) \leq 1.131 mc(G,w)\,.$$

PROOF. Let $\mathcal{C}$ denote the set of all odd cycles of G. Barahona (see [9]) proved that the solution of the max-cut problem for a nonnegatively weighted planar graph is given by the optimum solution of the following linear program (with variables x_e corresponding to edges of G):

$$\max \textstyle\sum_{e\in E} w_e x_e\ , \tag{28}$$

$$\textstyle\sum_{e\in C} x_e \leq |C|-1\,, \quad \text{for } C \in \mathcal{C}\ , \tag{29}$$

$$0 \leq x_e \leq 1\,, \qquad \text{for } e \in E\ . \tag{30}$$

Let us consider the dual linear program which reads

$$\min \textstyle\sum_{C\in\mathcal{C}}(|C|-1)\alpha_C + \sum_{e\in E}\beta_e\ , \tag{31}$$

$$\beta_e + \textstyle\sum\{\alpha_C \mid e\in C\in\mathcal{C}\} \geq w_e \quad \text{for } e\in E\,, \tag{32}$$

$$\alpha \geq 0, \quad \beta \geq 0 \tag{33}$$

where α_C ($C\in\mathcal{C}$) and β_e ($e\in E$) are dual variables corresponding to (29) and (30), respectively. Let α and β be the optimum dual solution. The dual constraint (32) can be interpreted as telling that the graph (G,w) is a subgraph of the amalgam of the collection of weighted odd cycles $\{(C,\alpha_C) \mid C\in\mathcal{C}\}$ and edges $\{(K_2,\beta_e) \mid e\in E\}$. Since the inequality $\varphi \leq 1.131mc$ holds for every member of the collection, it is true also for its amalgam (G,w) by the lemma. This proves the theorem. □

More detailed discussion about the relations between the linear programming and eigenvalue approach is given in [112]. The max-cut problem is polynomially solvable for nonnegatively weighted planar graphs by an exact algorithm [66, 104], and Theorem 2.13 shows that also eigenvalue approach provides a good estimate.

Another easy consequence of Lemma 2.12 is that

$$mc(G,w) = \varphi(G,w) \tag{34}$$

for arbitrary non-negatively weighted graphs, because each such graph can be built by the amalgamation of single edges, considered as weighted graphs (e,w_e). (It is $\varphi(K_2) = mc(K_2) = 1$.) Let us call a graph *exact* when the equality in (34) holds. It has been proved in [36] that the recognition of exact weighted graphs is an NP-complete problem. The status of complexity is open for unweighted exact graphs.

The bound $\varphi(G,w)$ has several properties analogous to $mc(G,w)$. We present them in the following theorems.

Let S be a subset of vertices of a weighted graph (G,w). The *switching* w^S of the weight function w is defined as

$$w^S_{ij} = \begin{cases} -w_{ij} & \text{for } ij\in\delta S \\ w_{ij} & \text{otherwise.} \end{cases}$$

The operation of switching was studied in a connection with the cut polytope. In particular, it is well known (and easy to check) that $mc(G,w^S) = mc(G,w) - w(\delta S)$. We show that φ has an analogous property.

THEOREM 2.14 *([36]) We have* $\varphi(G, w^S) = \varphi(G, w) - w(\delta S)$. □

The next operation that we consider is *vertex splitting*. Let $p_1, \ldots, p_n$ be integers. We define a weighted graph $(\tilde{G}, \tilde{w})$ by splitting each vertex i of G into p_i independent vertices $v_{i1}, \ldots, v_{ip_i}$, and the original weight w_{ij} is equally divided among the new edges p_ip_j between the splitted vertices, i.e., $\tilde{w}_{is,jt} = \frac{w_{ij}}{p_ip_j}$ for $i, j = 1, \ldots, n$, $s = 1, \ldots, p_i$, $t = 1, \ldots, p_j$. It is not difficult to see that $mc(\tilde{G}, \tilde{w}) = mc(G, w)$ for any splitting.

THEOREM 2.15 *([36]) We have* $\varphi(\tilde{G}, \tilde{w}) = \varphi(G, w)$ *for any splitting* $(\tilde{G}, \tilde{w})$ *of* (G, w). *Moreover, there exists an eigenvector* $\tilde{x}$ *corresponding to the optimized maximum eigenvalue of* $\varphi(\tilde{G}, \tilde{w})$ *such that the entries of* $\tilde{x}$ *coincide on each splitted vertex.* □

The splitting operation can be used to get an alternative definition of $\varphi(G, w)$, because for every nonnegatively weighted graph there (asymptotically) exists a splitting such that the optimum correcting vector for $(\tilde{G}, \tilde{w})$ is $u = 0$.

We define the *contraction* of a pair k and ℓ as follows. Let $G^{k\sim\ell}$ be the graph obtained from G by identifying vertices k and ℓ, and summing the weights on the identified edges. Formally, the vertex set of $G^{k\sim\ell}$ is $V(G)\backslash\{\ell\}$, and

$$w_{ij}^{k\sim\ell} = \begin{cases} w_{i\ell} + w_{ik} & \text{for } j = k \text{ (the identified vertex)} \\ w_{\ell j} + w_{kj} & \text{for } i = k \text{ (the identified vertex)} \\ w_{ij} & \text{for } i, j \notin \{k, \ell\} \ . \end{cases}$$

THEOREM 2.16 *([36]) We have* $\varphi(G^{k\sim\ell}, w^{k\sim\ell}) \leq \varphi(G, w)$ *for any contracted pair* k *and* ℓ. □

The operations of contraction and switching are useful in practical solving the max-cut problem by branch and bound technique. The contraction is used when a pair of nodes should be fixed in the same partition class. When two nodes i and j are fixed to belong to different classes, we first switch the weight function, and then consider the contraction of the pair i and j in the switched graphs. Theorems 2.14 and 2.16 ensure that the upper bound is nonincreasing in the branching process. Computational experiments with computing the upper bound $\varphi(G, w)$, and exactly solving the max-cut problem has been done by Poljak and Rendl [113]. A 'typical' gap between $mc(G, w)$ and $\varphi(G, w)$ is 4–5%.

2.5 Clustering

Stimulated by the work of Fiedler [45], Juhász and Mályusz [77] discovered an application of eigenvalue bounds to a clustering problem. The formulation of this problem is close to the bisection problem, but has a slightly different objective function. Let G be a (weighted) graph and A its (weighted) adjacency matrix. If $c = (S_1, S_2)$ is a partition of $V(G)$ into non-empty sets S_1, S_2 (called *clusters* of the partition c), denote by

$$f(c) = \frac{|S_1||S_2|}{|V(G)|}(d_{11} - 2d_{12} + d_{22})$$

where

$$d_{ij} = \frac{1}{|S_i||S_j|}\, e(S_i, S_j)\ , \quad i, j \in \{1, 2\}\,.$$

The task is to find a partition c for which $f(c)$ is maximum.

THEOREM 2.17 *([77]) Let G be a (weighted) graph of order n. Let P be the orthogonal projection parallel to $(1, \ldots, 1)^T$, i.e. $P = (\delta_{ij} - \frac{1}{n})$ where δ_{ij} is the Kronecker δ. Then*

$$f(c) \le \lambda_{\max}(PAP)$$

for any partition c of $V(G)$.

PROOF. We reproduce the proof (following [77]) since in [77] the theorem is proved for unweighted graphs only.

Given a partition $c = (S_1, S_2)$ of $V = V(G)$, let $x \in \ell^2(V)$ be the vector with coordinates

$$x_v = \begin{cases} \left(\frac{|S_2|}{|S_1||V|}\right)^{\frac{1}{2}} & \text{if } v \in S_1 \\ \\ -\left(\frac{|S_1|}{|S_2||V|}\right)^{\frac{1}{2}} & \text{if } v \in S_2\ . \end{cases}$$

Then $Px = x$ and $\|x\| = 1$. Moreover,

$$\begin{aligned} (PAPx, x) &= (Ax, x) = \sum_{u,v \in V} a_{uv} x_u x_v \\ &= \frac{|S_2|}{|S_1||V|} \sum_{u,v \in S_1} a_{uv} - \frac{2}{|V|} \sum_{u \in S_1, v \in S_2} a_{uv} + \frac{|S_1|}{|S_2||V|} \sum_{u,v \in S_2} a_{uv} \\ &= \frac{|S_1||S_2|}{|V|}(d_{11} - 2d_{12} + d_{22}) = f(c)\ . \end{aligned}$$

By the Rayleigh's principle (5) we get the inequality of the theorem. □

The functional f usually characterizes good clusterings. However, it is difficult to find an optimal partition. Therefore Juhász and Mályuzs [77, 75] proposed relaxations $F_1(c)$, $F_2(c)$, and $F_3(c)$ of $f(c)$, which can be easier optimized. A function $\rho \in \ell^2(V)$ is a *weight-function* if $\rho(v) \geq 0$ for $v \in V$ and $\sum_{v \in V} \rho(v)^2 = 1$. Then $\rho(v)$ can be viewed as the weight of the vertex v, and $\rho(v)\rho(u)$ is the weight of the edge vu. For $U \subseteq V$ define $\rho(U) = \sum_{u \in U} \rho(u)$, the weight of U. Then we define, for $c = (S_1, S_2)$:

$$F_1(c) = \max_{\rho(S_1)=\rho(S_2)} \{\rho(S_1)\rho(S_2)(d_{11}(\rho) - 2d_{12}(\rho) + d_{22}(\rho))\}$$

where

$$d_{ij}(\rho) = \frac{1}{\rho(S_i)\rho(S_j)} \sum_{u \in S_i} \sum_{v \in S_j} \rho(u)\rho(v)a_{uv} \ , \qquad i, j \in \{1, 2\}.$$

It is proved in [77] that $f(c) \leq F_1(c) \leq \lambda_{\max}(PAP)$. Further, it is shown that all optimal partitions for F_1 can be obtained by partitioning $V(G)$ according to the signs of coordinates of eigenvectors of PAP corresponding to its maximal eigenvalue.

The functional $F_2(c)$ is defined as an optimum over two weight-functions, δ and ρ:

$$F_2(c) = \min_{\delta} \max_{\rho} \left\{ \rho(S_1)\rho(S_2) \left(\frac{\rho(S_1)}{\rho(S_2)} d_{11}(\rho) - 2d_{12}(\rho) + \frac{\rho(S_2)}{\rho(S_1)} d_{22}(\rho) \right) \right\}$$

where the maximum is over all weight functions ρ such that $(\delta\rho)(S_1) = (\delta\rho)(S_2)$ with $(\delta\rho)(U) := \sum_{u \in U} \delta(u)\rho(u)$. Then ([77])

$$F_1(c) \geq F_2(c) \geq \lambda_{|V|-1}(A).$$

An optimal partition c with respect to F_2 can be obtained by the signs of the coordinates of the second largest eigenvalue $\lambda_{|V|-1}(A)$ of A.

The functional $F_3(c)$ is defined similarly:

$$F_3(c) = \min_{\rho} \left\{ \rho(S_1)\rho(S_2) \left(\frac{\rho(S_1)}{\rho(S_2)} d_{11}(\rho) - 2d_{12}(\rho) + \frac{\rho(S_2)}{\rho(S_1)} d_{22}(\rho) \right) \right\} .$$

One can prove ([76]) that

$$f(c) \geq F_3(c) \geq \lambda_{\min}(A)$$

and that an optimal partition c with respect to F_3 can be obtained by the signs of the coordinates of an eigenvector corresponding to $\lambda_{\min}(A)$. A behaviour of the clustering based on the above functionals for random graphs is studied in [76].

A clustering problem (with a fixed number $k \geq 2$ of clusters) was also studied by Bolla [17]. Let $v_1, \ldots, v_n$ be binary random variables taking values 0 and 1, and let $e'_1, \ldots, e'_m (m >> n)$ be a sample for the variables v_i. Then one can form a hypergraph $H = (V, E)$ with vertices $V = \{v_1, \ldots, v_n\}$ and hyperedges $E = \{e_1, \ldots, e_m\}$ where e_j contains all those vertices for which the value of the j-th object e'_j is equal 1. It is of practical interest [17] to partition E into k clusters, $E = E_1 \cup E_2 \cup \ldots \cup E_k$ such that the following criterion function is minimized:

$$Q = \sum_{i=1}^{k} Q(H_i)$$

where $H_i = (V_i, E_i)$ is the hypergraph corresponding to the i-th cluster E_i and

$$Q(H_i) = \min_{1 \leq d \leq n} \left\{ c \cdot 2^{n-d} + \sum_{j=1}^{d} \lambda_j(H_i) \right\}$$

with $c > 0$ a constant (its choice depends on the size of the problem), and $\lambda_j(H_i)$ the j-th eigenvalue of an appropriately defined Laplacian matrix $L(H)$ of the hypergraph H_i as described below. It is shown in [17] that the eigenvalue sum in $Q(H_i)$ is related to a combinatorial property of H_i. It measures how distinct the clusters H_i are from each other.

The Laplacian matrix $L(H)$ of a hypergraph $H = (V, E)$ on n vertices is defined by Bolla [17] as an $n \times n$ matrix with its ij-th entry ℓ_{ij} equal to

$$\ell_{ij} = \begin{cases} -\sum_{e \in E, v_i, v_j \in e} \frac{1}{|e|} & \text{if } i \neq j \\ \\ \sum_{e \in E, v_i \in e} \frac{|e|-1}{|e|} & \text{if } i = j \ . \end{cases}$$

Clearly, $|e|$ denotes the number of vertices incident with the hyperedge e. Note that if H is a graph then $L(H)$ defined above is equal to $\frac{1}{2}$ of the usual Laplacian matrix of the graph.

2.6 Graph partition

The graph partition problem asks for a partition of the vertex set of a weighted graph into a fixed number of classes of given sizes, so that the

number (resp. the weight) of edges between is minimum. Hence, the problem is a generalization of the bisection problem of section 2.1. The first eigenvalue bound on this problem is by Donath and Hoffman [42], which we recall in Theorem 2.21. Further work on the problem include [10, 11, 12, 13], where also several relaxation to the transportation problem were considered. We survey here only the recent results of Rendl and Wolkowicz [118] because they give the tightest eigenvalue bound.

The eigenvalue lower bound on the bisection width has been extended to a more general graph partition problem by Rendl and Wolkowicz [118]. The problem reads as follows.

Graph Partition Problem

Instance: A graph $G = (V, E)$, integers $m_1, \ldots, m_k$ such that $\sum_{i=1}^{k} m_i = n = |V|$.

Task: Find a partition $(S_1, \ldots, S_k)$ of V such that $|S_i| = m_i$, $i = 1, \ldots, k$, and the number of edges whose end vertices are in distinct partition classes is minimum.

Assume that $m_1, \ldots, m_k$ are fixed, and let $(S_1, \ldots, S_k)$ be an optimal partition. Let us denote by E_{cut} (and E_{uncut}) the set of edges whose endvertices belong to distinct classes (to the same class) of the partition. Let A denote the adjacency matrix of G. Let $\mathbf{1}_j = (1, \ldots, 1)^T$ be the all 1's vector of length j, and $m = (m_1, \ldots, m_k)^T$.

Theorem 2.18 *([118]) We have*

$$|E_{uncut}| \leq \min_u \max_x \frac{1}{2}\, tr(X^T(A + \mathrm{diag}(u))X)$$

where the minimum is taken over all vectors $u \in \boldsymbol{R}^n$ satisfying $\sum_{i=1}^{n} u_i = 0$, and the maximum is over all $n \times k$ matrices X satisfying

(i) $X\mathbf{1}_k = \mathbf{1}_n$,

(ii) $X^T\mathbf{1}_n = m$,

(iii) $X^T X = \mathrm{diag}(m)$.

Proof. Consider the matrix $X = (x_{ij})$ defined by $x_{ij} = 1$ if $i \in S_j$, and $x_{ij} = 0$ otherwise. It is straightforward to check that $|E_{uncut}| =$

$\frac{1}{2}\,tr(X^TAX)$, and X satisfies (i), (ii) and (iii). It is also easy to see that $tr(X^T\mathrm{diag}(u)X) = 0$ for any vector $u = (u_i)$ with $\sum_{i=1}^n u_i = 0$. □

The optimization problem formulated in Theorem 2.18 can be efficiently solved in two special cases, but a general solution is not known. The special cases are given in Corollaries 2.19 and 2.20. Let $Q = (q_1, \ldots, q_{n-1})$ be an $n \times (n-1)$ matrix whose columns $q_1, \ldots, q_{n-1}$ satisfy $q_i^T q_j = 0$ for $i \neq j$, $\|q_i\| = 1$ and $\mathbf{1}_n^T q_i = 0$ for $i = 1, \ldots, n-1$.

COROLLARY 2.19 *([118]) Let G be a graph with adjacency matrix A whose vertices are partitioned into sets of sizes $m_1, \ldots, m_k$, respectively, and let Q be a matrix as described above. Assume that $m_1 = \ldots = m_k = \frac{n}{k}$. Then $|E_{uncut}|$ is bounded above by*

$$\begin{aligned}&\min_u \max_X \left\{ \frac{1}{2}\, tr(X^T(A + \mathrm{diag}(u))X) \mid X \textit{ satisfies (i),(ii),(iii)} \right\} \\ &= \min_u \frac{n}{2k} \sum_{j=1}^{k-1} \lambda_{n-j+1}(Q^T(A + \mathrm{diag}(u))Q) + \frac{1}{k}|E| \qquad (35)\end{aligned}$$

where the minimum runs over all vectors $u \in \boldsymbol{R}^n$ with $\sum u_i = 0$.

Observe that Q^TAQ is of size $(n-1)\times(n-1)$, and hence $\lambda_{n-1}, \ldots, \lambda_{n-k+1}$ are the $k-1$ largest eigenvalues of Q^TAQ. We give the proof only for the special case of $k = 2$.

PROOF. Assume $m_1 = m_2 = \frac{n}{2}$. Then the conditions on X are equivalent with $X = (x, \mathbf{1}_n - x)$ where $x = (x_i)$ is a vector satisfying $\sum_{i=1}^n x_i = \sum_{i=1}^n x_i^2 = \frac{n}{2}$. Set $M = A + \mathrm{diag}(u)$, and $\mathbf{1} = \mathbf{1}_n$. We have

$$\begin{aligned}&\frac{1}{2}\, tr(X^TMX) = \frac{1}{2}(x^TMx + (\mathbf{1} - x)^TM(\mathbf{1} - x)) = \\ &x^TMx - \mathbf{1}^TMx + \frac{1}{2}\mathbf{1}^TM\mathbf{1} = \frac{1}{4}(\mathbf{1} - 2x)^TM(\mathbf{1} - 2x) + \frac{1}{4}\mathbf{1}^TM\mathbf{1}\ .\end{aligned}$$

Observe that

$$\frac{1}{4}\mathbf{1}^TM\mathbf{1} = \frac{1}{4}\mathbf{1}^TA\mathbf{1} + \frac{1}{4}\mathbf{1}^T\mathrm{diag}(u)\mathbf{1} = \frac{1}{2}|E| + \frac{1}{4}\sum_{i=1}^n u_i = \frac{1}{2}|E|.$$

Further, $y = \mathbf{1} - 2x$ satisfies $y^Ty = n$ by the properties of x. Hence

$$\min_X \frac{1}{2}\, tr(X^TMX) = \min_y \left\{ \frac{1}{4}y^TMy + \frac{1}{2}|E| \mid y^Ty = n \right\} = \frac{n}{4}\lambda_1(M) + \frac{|E|}{2}$$

by the Rayleigh's principle. □

The next corollary deals with the case of a 2-partition in possibly nonequal parts. Let $m_1 + m_2 = n$, and denote

$$\begin{aligned} C(u) &= \frac{1}{n} m_1 m_2 \, Q^T (A + \mathrm{diag}(u)) Q \ , \\ c(u) &= \frac{m_1 - m_2}{n} \sqrt{\frac{m_1 m_2}{n}} \, Q^T (A + \mathrm{diag}(u)) Q \ , \\ c' &= |E| (m_1^2 + m_2^2) \frac{1}{2n^2} \, . \end{aligned}$$

COROLLARY 2.20 *([118]) Suppose we have a 2-partition of $V(G)$ into sets of sizes m_1 and m_2, respectively. Then $|E_{uncut}|$ is bounded above by*

$$\min_u \max_X \left\{ \frac{1}{2} \, tr(X^T (A + \mathrm{diag}(u)) X) \mid X \text{ satisfies (i),(ii),(iii)} \right\} =$$
$$\min_u \max_z \left\{ z^T C(u) z + c(u)^T z + c' \mid z \in \boldsymbol{R}^{n-1}, \|z\| = 1 \right\}$$

where the minimum runs over all vectors $u \in \boldsymbol{R}^n$ with $\sum u_i = 0$. □

Both Corollaries 2.19 and 2.20 can be viewed as generalizations of the Boppana's bound of Corollary 2.3. This can be shown as follows. By Corollary 2.19 (or 2.20) we have (with $U = \mathrm{diag}(u)$)

$$|E_{uncut}| \leq \min_u \frac{n}{4} \lambda_{\max}(Q^T (A + U) Q) + \frac{|E|}{2} \ ,$$

and hence

$$|E_{cut}| = |E| - |E_{uncut}| \geq \frac{|E|}{2} - \frac{n}{4} \min_u \lambda_{\max}(Q^T (A + U) Q).$$

Let $\overline{d} = \sum d_i / n = 2|E|/n$ denote the average vertex degree of G. Then

$$\frac{|E|}{2} - \frac{n}{4} \lambda_{\max}(Q^T (A + U) Q) = \frac{n}{4} \lambda_{\min}(\overline{d} I_{n-1} - Q^T (A + U) Q) =$$
$$\frac{n}{4} \lambda_{\min}(Q^T (\overline{d} I_n - A - U) Q) = \frac{n}{4} \lambda_{\min}(Q^T (D - A + \mathrm{diag}\ (u')) Q)$$

where $D = \mathrm{diag}(d_1, \ldots, d_n)$ is the diagonal matrix defined by the degrees of the graph G, and $u'_i = \overline{d} - d_i - u_i$, $i = 1, \ldots, n$. Observe that $\sum u'_i = \sum u_i + n\overline{d} - \sum d_i = \sum u_i = 0$, and $L = D - A$ is the Laplacian matrix of G. This proves the equivalence of the bounds.

A bound on the general graph partition problem has already been formulated by Donath and Hoffman in [42].

THEOREM 2.21 *([42]) Assume that $m_1 \geq m_2 \geq \ldots \geq m_k$. Then*

$$|E_{cut}| \geq \max_u \frac{1}{2} \sum_{i=1}^{k} m_i \lambda_i(L(G) + \mathrm{diag}(u)) \tag{36}$$

where the maximum runs over all vectors $u \in \boldsymbol{R}^n$ with $\sum u_i = 0$. □

However, the bound given by this theorem is weaker than that of Theorem 2.18. It should be mentioned that Donath and Hoffman derived another partition result [42, Theorem 3].

3 Ordering

A number of recent papers use eigenvalues and eigenvectors of matrices associated to graphs to obtain orderings (labellings) of vertices of a graph which give rise to acceptable approximations for several optimization problems on graphs. Applications to cutwidth, bandwidth and the min-p-sum problem use the Laplacian matrix, its second smallest eigenvalue and the corresponding eigenvectors. Applications to ranking and scaling use the Perron-Frobenius eigenvector.

3.1 Bandwidth and min-p-sum problems

A *labelling* of a (weighted) graph $G = (V, E)$ is a 1-1 mapping $\psi : V \to \{1, \ldots, |V|\}$. For a real number p, $0 < p < \infty$, we define its *p-discrepancy* $\sigma_p(G, \psi)$ as

$$\sigma_p(G, \psi) := \Big(\sum_{uv \in E} a_{uv} |\psi(u) - \psi(v)|^p \Big)^{1/p},$$

and for $p = \infty$,

$$\sigma_\infty(G, \psi) := \max_{uv \in E} |\psi(u) - \psi(v)|.$$

Notice that $\sigma_\infty(G, \psi)$ is independent of the edge weights a_{uv}. The minimal value

$$\sigma_p(G) := \min_\psi \sigma_p(G, \psi), \qquad 0 < p \leq \infty,$$

is called the *min-p-sum* of the graph G. For the case $p = \infty$, $\sigma_\infty(G)$ is also known as the *bandwidth* of the graph G. The reader can find more information about the min-1-sum and the bandwidth in [27, 26]. Let us just

mention that the bandwidth and the min-1-sum problem are NP-complete in general [54, 110].

As for the comments in the introduction, good lower bounds on $\sigma_p(G)$ are extremely important and nontrivial to obtain. Let us present a result of Juvan and Mohar [79].

THEOREM 3.1 *([79]) Let G be a graph of order n with at least one edge, and let*

$$\beta(G) := \sup_w \left\lceil \frac{n}{\lambda_2(G_w)} \left(-\Delta(G_w) + \sqrt{\Delta^2(G_w) + \lambda_2^2(G_w)} \right) \right\rceil$$

where the supremum is taken over all non-negative weightings w of the edges of G, and where $\lambda_2(G_w)$ is the second smallest eigenvalue of the corresponding weighted Laplacian matrix and $\Delta(G_w)$ denotes the maximal w-weighted degree of G. Then

$$\sigma_\infty(G) \geq \begin{cases} \beta(G) - 1 & \text{if } \beta(G) \equiv n \ (mod\, 2) \\ \beta(G) & \text{otherwise.} \end{cases}$$

PROOF. We will use the separation result of Section 2.2. Fix an arbitrary weighting function w, and let $\lambda_i = \lambda_i(G_w)$. Also, choose an optimal labelling ψ for the bandwidth of G. Define $A, B, C \subset V(G)$ as follows:

$$\begin{aligned} A &:= \{v \in V(G) \mid \psi(v) \leq (n-k)/2\} \\ B &:= \{v \in V(G) \mid \frac{n-k}{2} < \psi(v) \leq (n+k)/2\} \\ C &:= \{v \in V(G) \mid \psi(v) > (n+k)/2\} \end{aligned}$$

where $1 \leq k < n$ is a number to be determined later. We will assume that $k \equiv n \ (mod\, 2)$. Notice that $|A| = |C| = (n-k)/2$ and $|B| = k$. The sum of the weights of the edges between particular parts A, B, C can be estimated using Proposition 2.6 as follows:

$$e(A, B \cup C) \geq \lambda_2 \frac{|A|\,|B \cup C|}{n} \tag{37}$$

$$e(A \cup B, C) \geq \lambda_2 \frac{|C|\,|A \cup B|}{n} \tag{38}$$

$$e(B, A \cup C) \leq \Delta |B| \ . \tag{39}$$

Since

$$2e(A, C) = e(A, B \cup C) + e(A \cup B, C) - e(B, A \cup C) \tag{40}$$

we get from (37)–(39) that

$$2e(A,C) \geq \frac{\lambda_2}{2n}(n^2 - k^2) - \Delta k \ . \tag{41}$$

It follows that $e(A,C) > 0$ if $k < \frac{n}{\lambda_2}(-\Delta + \sqrt{\Delta^2 + \lambda_2^2})$ which implies that there is at least one edge between A and C. Consequently, $\sigma_\infty(G) \geq k+1$ where

$$k := \left\lceil \frac{n}{\lambda_2}\left(-\Delta + \sqrt{\Delta^2 + \lambda_2^2}\right)\right\rceil - \varepsilon$$

and $\varepsilon = 1$ or 2 (chosen so that $k \equiv n \ (mod\, 2)$). □

Notice that if λ_2 is small compared to Δ, the lower bound of Theorem 3.1 behaves like $\lambda_2 n/(2\Delta)$ and for $\lambda_2 = \Delta(1 - o(1))$ it behaves like $(\sqrt{2} - 1)n(1 - o(1))$. If we replace the inequality (39) with

$$e(B, A \cup C) \leq \lambda_n \frac{k(n-k)}{n} \tag{42}$$

(cf. Proposition 2.7) we get another lower bound [79] on the bandwidth:

$$\sigma_\infty(G) \geq \begin{cases} \beta'(G) - 1 & \text{if } \beta'(G) \equiv n \ (mod\, 2) \\ \beta'(G) & \text{otherwise} \end{cases} \tag{43}$$

where $\beta'(G)$ is defined as

$$\beta'(G) := \sup_w \left\lceil \frac{\lambda_2(G_w)}{2\lambda_n(G_w) - \lambda_2(G_w)}\, n \right\rceil \ . \tag{44}$$

The supremum is again over all non-negative edge weighting functions w. It is easy to see that the supremum in the definitions of $\beta(G)$ and $\beta'(G)$ is always attained. Unfortunately, unlike some other similar optimizations (cf. Sections 2 and 4) we do not know of an efficient algorithm for computing $\beta(G)$ or $\beta'(G)$.

Further improvements are possible. The first possibility is to use in (37) and (38) improved bounds on partitions as outlined in Sections 2.1 and 2.2. Another approach has the following background. It may happen that $\lambda_2(G_w) = 0$ for every weighting w and therefore also $\beta'(G) = 0$ (and $\beta(G) = 0$ with the proper interpretation). Of course, this will happen if and only if G is disconnected. Well, if one of the components of G is large, the others very small, the bandwidth will depend on the large component.

One may assume that in such a case we reduce the bandwidth problem to the connected components. However, the same will happen if there is a small part of the graph which is "loosely" connected to the rest. Possible improvements will be to add (weighted) edges to the graph in order to get rid of such such anomalies. The proof of Theorem 3.1 will go through with the same arguments. The only difference will be to replace the condition $e(A, C) > 0$ with

$$e(A, C) > w^+ := \sum_{uv \notin E(G)} w(uv)\,. \tag{45}$$

In this case we get the bound:

$$\sigma_\infty(G) \geq \left\lceil \frac{n}{\lambda_2} \left(-\Delta_w + \sqrt{\Delta_w^2 + \lambda_2(\lambda_2 - 2w^+/n)} \right) \right\rceil - 1$$

where $\lambda_2 = \lambda_2(G_w)$ and $\Delta_w = \Delta(G_w)$ is the maximal (weighted) degree of G_w. There is a similar bound along the lines of (43) and (44).

There is another possibility of optimization. One may try to find a subgraph G' of G for which any of the previous bounds will be better than for G. It is obvious by the Courant-Fisher principle that $\lambda_{\max}(G') \leq \lambda_{\max}(G)$ but it may happen that $\lambda_2(G') > \lambda_2(G)$ if G contains fewer vertices than G.

In [78] also bounds on $\sigma_1(G)$ and $\sigma_2(G)$, the most useful among the parameters $\sigma_p(G)$, $0 < p < \infty$, are obtained.

THEOREM 3.2 *([78]) Let G be a (weighted) graph of order n and let $\overline{d}(G)$ denote the average (weighted) degree of G. Then*

$$(a) \qquad \lambda_2(G)\frac{n^2-1}{6} \leq \sigma_1(G) \leq \overline{d}(G)\frac{n(n+1)}{6}\,,$$

$$(b) \qquad \lambda_2(G)\frac{n(n^2-1)}{12} \leq \sigma_2(G)^2 \leq \overline{d}(G)\frac{n^2(n+1)}{12}\,.$$

□

Juvan and Mohar [78] suggested to use eigenvectors corresponding to $\lambda_2(G)$ to determine an approximation to an optimal labelling for any of the problems of calculating $\sigma_p(G)$, $0 < p \leq \infty$. Their calculations on several classes of graphs show fairly successful behaviour. A labelling corresponding to a vector $x \in \ell^2(V(G))$ is determined by the increase of components $x_v, v \in$

$V(G)$, of x. The vertex v with the smallest value x_v will be labelled 1, the second smallest 2, etc. The heuristic argument behind this algorithm is that eigenvectors of $\lambda_2(G)$ minimize the sum $\sum_{uv\in E}(x_u - x_v)^2$ (under the constraint $x^t\mathbf{1} = 0$, $\|x\| = 1$ which guarantee that x is not a "multiple of $\mathbf{1}$"), and $\sigma_2(G)$ minimizes $\sum_{uv\in E}(\psi(u) - \psi(v))^2$.

3.2 Cutwidth

The *cutwidth* $c(G)$ of a (weighted) graph G of order n is defined as the minimum of $c(G,\psi)$ over all labellings ψ of G where

$$c(G,\psi) = \max_{1\le i<n} e(\psi^{-1}(\{1,2,\ldots,i\}), \psi^{-1}(\{i+1,\ldots,n)\}).$$

In other words, we want a labelling ψ where the maximal number (sum of the weights) of edges between vertices with $\psi(v) \le i$ and vertices with $\psi(u) > i$ $(1 \le i < n)$, is as small as possible. It is known that the cutwidth computation is NP-hard [53]. The following simple result is outlined in [78]:

THEOREM 3.3 *([78]) Let G be a graph of order n and ψ a labelling of G. Then*

$$\lambda_2(G)\frac{\lfloor\frac{n}{2}\rfloor\lceil\frac{n}{2}\rceil}{n} \le c(G,\psi) \le \lambda_n(G)\frac{\lfloor\frac{n}{2}\rfloor\lceil\frac{n}{2}\rceil}{n}.$$

Consequently,

$$\lambda_2(G)\frac{\lfloor\frac{n}{2}\rfloor\lceil\frac{n}{2}\rceil}{n} \le c(G) \le \lambda_n(G)\frac{\lfloor\frac{n}{2}\rfloor\lceil\frac{n}{2}\rceil}{n}.$$

□

3.3 Ranking

An idea of using eigenvalues and eigenvectors for the tournament ranking problem appears in the book of Berge [14]. Let $G = (V,F)$ be a *partial tournament*, i.e., a directed graph such that $ij \in F$ implies that $ji \notin F$. The existence of an arc ij means that the player i has beaten the player j. One can rank the players in a partial tournament using the outdegrees (number of wins). But it may happen that "while one player has beaten a large number of very weak players, another player has beaten only a few very strong players." To discover such "anomalies" one can use quite successfully the following ranking procedure based on the *power indices* as defined below.

Let $p_i^j(k)$ denote the number of walks of length k from the vertex i to j, and let

$$p^j(k) = p_1^j(k) + \cdots + p_n^j(k)$$

where $n = |V|$ as usual. The *power index* of the j-th player is defined as

$$\pi^j = \lim_{k\to\infty} \frac{p^j(k)}{p^1(k) + \cdots + p^n(k)} \ .$$

THEOREM 3.4 *The power indices of players in a partial tournament are given by the positive eigenvector of the adjacency matrix of the tournament normalized in the ℓ^1-norm.*

PROOF. It is well-known that the entries of the k-th power of the adjacency matrix A determine the number of walks of length k, i.e. $A^k = [p_i^j(k)]_{i,j\in V}$. Therefore $p^j(k) = e_j A^k \mathbf{1}$ where e_j is the vector with j-th coordinate equal to 1, all others equal to 0. By the Perron-Frobenius theorem, A has a positive eigenvector, and its eigenvalue has the largest modulus among the eigenvalues of A. Moreover, by the power method, $A^k\mathbf{1}/\|A^k\mathbf{1}\|$ converges to the Perron-Frobenius eigenvector. Therefore also a different normalization $A^k\mathbf{1}/\mathbf{1}A^k\mathbf{1}$, which approaches the vector of power indices, converges to a multiple of the normalized Perron-Frobenius eigenvector. □

Applications in geography. Similar idea appeared also in the geographic literature, where it was used to compare accessibility of nodes in a transportation network. The accessibility of a node i is expressed by its index (called *Gould index*) π^i defined by

$$\pi^i = \frac{x_i}{\|x\|}$$

where x is the eigenvector of $\lambda_{\max}(A(G))$ and G is an undirected graph representing the network. The references to applications can be found in the survey paper [127].

3.4 Scaling

A method of scaling based on the maximum eigenvector has been proposed by T. L. Saaty in [121]. A matrix $A = (a_{ij})$ is *positive and reciprocal* if $a_{ij} = a_{ji}^{-1} > 0$ for $i, j = 1, \ldots, n$. The goal is to find a positive vector

$w = (w_1, \ldots, w_n)$, called a *scaling*, so that the entries a_{ij} of A are, in some sense, well approximated by the ratios $\frac{w_i}{w_j}$. This will be denoted as $a_{ij} \approx \frac{w_i}{w_j}$.

In practical applications, the matrix A may be obtained as a matrix of pairwise comparisons, and the entries a_{ij} are obtained by consulting a board of experts. As a heuristical method of scaling, T. L. Saaty proposed to take the eigenvectors corresponding to the maximum eigenvalue $\lambda_{\max}(A)$. By the Perron-Frobenius theorem, this eigenvector is unique, and all its entries are positive. T. L. Saaty has shown the following properties of w.

THEOREM 3.5 *([121]) Let A be a positive reciprocal matrix of size $n \times n$ and w its Perron-Frobenius eigenvector. Then the following holds:*

(i) $\lambda_{\max}(A) \geq n$,

(ii) $\lambda_{\max}(A) = n$ *if and only if* $a_{ij}a_{jk} = a_{ik}$ *for all* $i, j, k = 1, \ldots, n$ *(i.e., A is already scaled).*

(iii) If $a_{1j} \leq a_{2j} \leq \ldots \leq a_{nj}$ *for all* j, *then* $w_1 \leq w_2 \leq \ldots \leq w_n$.

PROOF. (i) Since $\lambda_{\max}$ is the eigenvalue with the eigenvector w, we have

$$\sum_{j=1}^{n} a_{ij} w_j = \lambda_{\max}\, w_i, \quad i = 1, \ldots, n,$$

which gives

$$\sum_{i=1}^{n} \sum_{j=1}^{n} a_{ij} w_j w_i^{-1} = n\lambda_{\max}\ .$$

Applying the inequality $x + 1/x \geq 2$ with $x = a_{ij}w_j w_i^{-1}$, we get $x + 1/x = a_{ij}w_j w_i^{-1} + a_{ji}w_i w_j^{-1} \geq 2$, which together with $a_{ii} = 1$ gives

$$\begin{aligned} n\lambda_{\max} &= \sum_{i,j=1}^{n} a_{ij} w_j w_i^{-1} \\ &= \sum_{i=1}^{n} a_{ii} + \sum_{1 \leq i < j \leq n} (a_{ij} w_j w_i^{-1} + a_{ji} w_i w_j^{-1}) \geq n + 2\binom{n}{2} = n^2\ . \end{aligned}$$

Hence $\lambda_{\max} \geq n$.

(ii) It follows from the above inequality that $\lambda_{\max} = n$ if and only if $x + 1/x = a_{ij}w_j w_i^{-1} + a_{ji}w_i w_j^{-1} = 2$, for all pairs i, j. This holds only if

$a_{ij}w_j w_i^{-1} = 1$ for all $i, j = 1, \ldots, n$, and this is equivalent to the condition in (ii).

(iii) Fix $i < j$. Since $w_k > 0$, and $a_{ik} \leq a_{jk}$ for $k = 1, \ldots, n$, we have

$$\lambda_{\max} w_i = \sum_{k=1}^{n} a_{ik} w_k \leq \sum_{k=1}^{n} a_{jk} w_k = \lambda_{\max} w_j \ .$$

Hence $w_i \leq w_j$. □

Parts (i) and (ii) of Theorem 3.5 indicate that the difference between $\lambda_{\max}$ and n depends on how far the matrix A is from a scaled matrix. In fact, Saaty [121] has shown that the value of $(\lambda_{\max} - n)/(n-1)$ corresponds to the variance of $\varepsilon_{ij} = a_{ij} w_j w_i^{-1}$.

3.5 The quadratic assignment problem

The quadratic assignment problem is one of the most interesting combinatorial optimization problems, with many applications in the layout theory. Several other known hard combinatorial optimization problems, like the travelling salesman, the bisection width, or the min-1-sum problem are special cases of the quadratic assignment problem. (The bisection width and the min-1-sum problem are considered in Sections 2.1 and 3.1, respectively.) The problem reads as follows.

Quadratic Assignment Problem

Instance: Matrices A, B and C of size $n \times n$.

Task: Find a permutation π of $\{1, 2, \ldots, n\}$ which minimizes

$$\sum_{i=1}^{n} c_{i\pi(i)} + \sum_{i=1}^{n} \sum_{j=1}^{n} a_{ij} b_{\pi(i)\pi(j)} \ . \tag{46}$$

The crucial application of the eigenvalue approach is estimating the quadratic term in (46). The following theorem, concerning the symmetric case, is due to Finke, Burkard, and Rendl [48].

Theorem 3.6 *([48]) Let A and B be symmetric $n \times n$ matrices with eigenvalues $\lambda_1 \leq \ldots \leq \lambda_n$ and $\mu_1 \leq \ldots \leq \mu_n$, respectively. Then*

$$\min_{\pi} \sum_{i=1}^{n} \sum_{j=1}^{n} a_{ij} b_{\pi(i)\pi(j)} \geq \sum_{i=1}^{n} \lambda_i \mu_{n-i+1} \tag{47}$$

where the minimum is taken over all permutations π *of* $\{1, 2, \ldots, n\}$.

PROOF. Let π be the permutation which realizes the minimum in (47), and let X be the permutation matrix corresponding to π. Since B and XBX^T are similar, the eigenvalues of XBX^T are also $\mu_1 \leq \ldots \leq \mu_n$. We have

$$\sum_{i=1}^{n}\sum_{j=1}^{n} a_{ij}b_{\pi(i)\pi(j)} = tr(AXBX^T)$$

and using the Hoffman-Wielandt inequality (15) we finally get:

$$tr(A(XBX^T)) \geq \sum_{i=1}^{n} \lambda_i \mu_{n-i+1} \ .$$

□

Further results and generalizations to non-symmetric case appear in [63, 64, 117]. A survey of applications of the quadratic assignment problem is in [23].

4 Stable sets and coloring

In this section we survey eigenvalue bounds on the chromatic number $\chi(G)$ and the size of a maximum stable set $\alpha(G)$. The lower bound on $\chi(G)$ (due to A. Hoffman [67]), and the upper bound on $\chi(G)$ (due to H. Wilf [132]) are probably the earliest applications of spectral bounds to a graph optimization problem. On the other hand, theoretically most important is the Lovász's bound $\vartheta(G)$ on the maximum stable set size.

We recall that the *chromatic number* $\chi(G)$ is the minimum number of colors needed to color the vertices of G so that no two adjacent vertices have the same color. A set S is called *stable* or *independent* if no two vertices of S are adjacent. The maximum size of a stable set is denoted by $\alpha(G)$. We let $\overline{G}$ denote the complement of G. The coloring and the stable set problems make sense only for simple graphs. Therefore all graphs in this section are assumed to be simple.

4.1 Chromatic number

The first eigenvalue bounds on the chromatic number are due to H. Wilf [132] and A. Hoffman [67] who formulated an upper and a lower bound, respectively.

THEOREM 4.1 *([132, 67]) Let $A = A(G)$ be the adjacency matrix of a simple graph G. Then*

$$1 + \frac{\lambda_{\max}(A)}{|\lambda_{\min}(A)|} \leq \chi(G) \leq 1 + \lambda_{\max}(A) \ . \tag{48}$$

PROOF. (See [133].) Let G_{crit} be a maximal color-critical subgraph of G (i.e. a subgraph of G with the same chromatic number and such that deleting any edge decreases the chromatic number). Let d denote the minimum degree of G_{crit}. We have

$$\chi(G) - 1 \leq d \leq \lambda_{\max}(A(G_{crit})) \leq \lambda_{\max}(A(G)) \ .$$

A short proof of the lower bound, based on the interlacing property of eigenvalues, can be found in [55] or [86]. □

Let us remark that the upper bound can be realized by an efficient algorithm, i.e., one can color any graph G by $1 + \lambda_{\max}(A(G))$ colors in polynomial time. (This question was raised in [8].) The algorithm follows from an easy lemma (see, e.g., [34]).

LEMMA 4.2 *The average degree $\overline{d}$ of G is less or equal to $\lambda_{\max}(A(G))$.* □

Let v_1 be a vertex of G whose degree is at most the average degree $\overline{d}$. Clearly, such a vertex can easily be found. By the interlacing property of eigenvalues, $\lambda_{\max}(A(G - v_1)) \leq \lambda_{\max}(A(G))$. Assume that $G - v_1$ is already colored with at most $k = \lfloor 1 + \lambda_{\max}(A(G)) \rfloor$ colors. Since the degree of v_1 is at most $k - 1$, the coloring can be extended to G. This gives a polynomial time algorithm.

The following two theorems are due to Cvetković [32] and Hoffman [67].

THEOREM 4.3 *([32, 34]) Let G be a simple graph of order n. Then*

$$\chi(G) \geq \frac{n}{n - \lambda_{\max}(A(G))} \ .$$

THEOREM 4.4 *([67]) Let G be a simple graph of order n distinct from the complete graph K_n, and let $\overline{G}$ denote the complement of G. Then*

$$\chi(\overline{G}) \geq \frac{n + \lambda_{n-1}(A(G)) - \lambda_n(A(G))}{1 + \lambda_{n-1}(A(G))} \ .$$

Eigenvectors can also be used to obtain a coloring of a graph. In fact, bipartite graphs are fully characterized by the following theorem.

THEOREM 4.5 *([34], Theorems 3.4 and 3.11) A graph G is bipartite if and only if*

$$\lambda_{\min}(A(G)) = -\lambda_{\max}(A(G)) \ .$$

□

The bipartition of a bipartite graph G is given by the sign-pattern of an eigenvector corresponding to $\lambda_{\min}(A(G))$. The idea has been extended by Apswall and Gilbert [8] to obtain a heuristic graph coloring algorithm using the following result as the basis of the heuristic. Let $x_1, \ldots, x_r$ be a collection of vectors from $\boldsymbol{R}^n$. The vectors $x_\ell = (x_{1\ell}, \ldots, x_{n\ell})$, $\ell = 1, \ldots, r$, determine a partition (i.e. coloring) of $\{1, \ldots, n\}$ as follows. Let i and j belong to the same partition class if and only if either $x_{i\ell} \geq 0$ and $x_{j\ell} \geq 0$ for $\ell = 1, \ldots, r$, or $x_{i\ell} < 0$ and $x_{j\ell} < 0$ for $\ell = 1, \ldots, r$. In other words, the partition classes are given by the sign-patterns of the collection (where the zero entries are considered as positive).

THEOREM 4.6 *([8]) Let $x_1, \ldots, x_n$ be pairwise orthogonal eigenvectors of $\lambda_1(A(G)), \ldots, \lambda_n(A(G))$, respectively. Then, for every pair i and j of adjacent vertices, there exits an eigenvector x_ℓ for which $x_{i\ell}$ and $x_{j\ell}$ have distinct signs.*

In some cases, the minimum coloring can be obtained via sign-pattern of a collection of vectors. An explicit class of graphs is given in Theorem 4.7. A graph $G = (V, E)$ is called *block regular k-partite*, if (i) G is a k-partite graph with partition $V = V_1 \cup \ldots \cup V_k$, and (ii) for every $i, j, i \neq j$, the number of edges from a vertex $u \in V_i$ to V_j depends only on i and j.

THEOREM 4.7 *([8]) Let G be a block regular k-partite graph. Then there exists a set of at most $k-1$ eigenvectors whose sign-pattern induces a proper k-coloring of G.* □

For ideas of the similar flavor we also refer to [115, 116].

4.2 Lower bounds on stable sets

H. S. Wilf [134] derived a spectral bound on the size of the maximum stable set using an earlier result of Motzkin and Straus [101].

THEOREM 4.8 *([134]) Let G be a simple graph. Then*

$$\alpha(G) \geq \frac{s^2}{s^2 - \lambda_{\max}(A(\overline{G}))}$$

where s is the sum of entries of the normalized eigenvector corresponding to $\lambda_{\max}(A(\overline{G}))$.

PROOF. Let $G = (V, E)$ be a graph with vertex set $V = \{1, \ldots, n\}$. We need a result of Motzkin and Straus [101], who proved that $\alpha(G)$ can be expressed as an optimum of a quadratic program as follows:

$$\max \left\{ \sum_{ij \notin E} x_i x_j \mid \sum_{i=1}^{n} x_i = 1, x \geq 0 \right\} = 1 - \frac{1}{\alpha(G)} \ .$$

Let $u = (u_i) \geq 0$ be the normalized eigenvector corresponding to the eigenvalue $\lambda_{\max}(A(\overline{G}))$, and let $s := \sum_{i=1}^{n} u_i$. Then $y = u_i/s$ satisfies $y \geq 0$ and $\sum_{i=1}^{n} y_i = 1$, and hence

$$1 - \frac{1}{\alpha(G)} \geq \sum_{ij \notin E} y_i y_j = y^T A(\overline{G}) y = \lambda_{\max}(A(\overline{G}))\|y\|^2 = \frac{1}{s^2}\lambda_{\max}(A(\overline{G})).$$

□

COROLLARY 4.9 *([134]) For a simple graph G we have*

$$\alpha(G) \geq \frac{n}{n - \lambda_{\max}(A(\overline{G}))}.$$

PROOF. It follows from the fact that $s^2 \leq n$. □

Corollary 4.9 generalizes the bound of Cvetković given in Theorem 4.3, since

$$\chi(G) \geq \alpha(\overline{G}) \geq \frac{n}{n - \lambda_{\max}(A(G))}.$$

In fact, H. S. Wilf derived a hierarchy of spectral bounds. One of them is given in the next theorem.

THEOREM 4.10 *([134]) Let G be a d-regular graph on n vertices. Then*

$$\alpha(G) \geq \frac{n}{d + 1 + (\lambda_{\min}(A(G)) + 1)\max(M_+^2, M_-^2)/n}$$

where $M_+ = \min_{u_i > 0} \frac{1}{u_i}$, $M_- = \min_{u_i < 0} \frac{1}{|u_i|}$, and u is the normalized eigenvector of the second largest eigenvalue of $A(G)$. □

4.3 Upper bounds on stable sets

L. Lovász introduced an eigenvalue bound $\vartheta(G)$ on $\alpha(G)$ in the connection with his solution of the problem of Shannon capacity of the 5-cycle, see [85]. Given a graph $G = (V, E)$, the number $\vartheta(G)$ is defined by

$$\vartheta(G) := \min_{A \in \mathcal{A}} \lambda_{\max}(A) \tag{49}$$

where $\mathcal{A}$ is the class of real $n \times n$ matrices $A = (a_{ij})$, where $n = |V|$, satisfying

$$a_{ij} = \begin{cases} 1 & \text{for } ij \notin E, \text{ or } i = j, \\ \text{arbitrary} & \text{otherwise.} \end{cases} \tag{50}$$

THEOREM 4.11 *([85]) For every graph G, we have $\alpha(G) \leq \vartheta(G)$.*

PROOF. Let $k = \alpha(G)$ and let S be a stable set of size $k = \alpha(G)$. Assume that $A \in \mathcal{A}$ is a matrix for which $\lambda_{\max}(A) = \vartheta(G)$. (It is easy to see that the minimum in (49) is attained.) Define a vector $y = (y_i)$, $\|y\| = 1$, by

$$y_i = \begin{cases} k^{-1/2} & \text{for } i \in S \\ 0 & \text{otherwise.} \end{cases} \tag{51}$$

Then

$$\alpha(G) = k = y^T A y \leq \max_{\|x\|=1} x^T A x = \lambda_{\max}(A) = \vartheta(G)\,.$$

□

Important is the dual characterization of $\vartheta(G)$.

THEOREM 4.12 *([85]) Let $\mathcal{B}$ denote the class of positive semidefinite symmetric matrices $B = (b_{ij})$ satisfying $\sum_{i=1}^{n} b_{ii} = 1$ and $b_{ij} = 0$ for i and j adjacent. Then*

$$\vartheta(G) = \max_{B \in \mathcal{B}} \sum_{i,j} B_{i,j}.$$

□

Lovász gives also several other equivalent definitions of $\vartheta(G)$.

THEOREM 4.13 *([85]) We have*

$$\vartheta(G) = \max_{B \in \mathcal{B}} \left(1 - \frac{\lambda_{\max}(B)}{\lambda_{\min}(B)}\right)$$

where $B \in \mathcal{B}$ if and only if $b_{ij} = 0$ for $ij \in E$ and for $i = j$, and b_{ij} is arbitrary otherwise. □

Lovász also proves that $\chi(G) \geq \vartheta(\overline{G})$, and hence Theorem 4.13 yields the Hoffman's lower bound on $\chi(G)$ presented in Theorem 4.1.

The number $\vartheta(G)$ is probably the best known efficiently computable estimate of $\alpha(G)$. Moreover, $\alpha(G) = \vartheta(G)$ for perfect graphs. However, there is a big gap between the performance of $\alpha(G)$ and $\vartheta(G)$ on random graphs. It is well known that $\alpha(G) \approx 2 \ln n$. On the other hand, Juhász [73] determined $\vartheta(G)$ for random graphs.

THEOREM 4.14 *([73]) Let G be a random graph with edge probability $p = 1/2$. Then, with probability $1 - o(1)$ for $n \to \infty$,*

$$\frac{1}{2}\sqrt{n} + O(n^{1/3} \log n) \leq \vartheta(G) \leq 2\sqrt{n} + O(n^{1/3} \log n) .$$

□

4.4 k-colorable subgraphs

Narasimhan and Manber [102] recently extended the eigenvalue bound $\vartheta(G)$ to obtain a bound on the maximum size of a k-colorable subgraph.

Given a graph $G = (V, E)$, let $\alpha_k(G)$ denote the maximum size of a k-colorable subgraph of G, i.e.

$$\alpha_k(G) = \max\{|S_1 \cup \ldots \cup S_k| \ : \ S_i \text{ is stable, } i = 1, \ldots, k\} .$$

Let $\mathcal{A}$ be the class of matrices defined by (50). Let

$$\vartheta_k(G) := \min \left\{ \sum_{i=1}^{k} \lambda_{n-i+1}(A) \mid A \in \mathcal{A} \right\}$$

i.e., $\vartheta_k(G)$ is the sum of the k largest eigenvalues of $A \in \mathcal{A}$, where A is chosen so that the sum in minimized. The bound $\vartheta_k(G)$ improves the obvious bound $\alpha_k(G) \leq k\vartheta(G)$.

THEOREM 4.15 *([102]) We have $\alpha_k(G) \leq \vartheta_k(G)$ for every graph G.*

PROOF. The proof is quite analogous to that of Theorem 4.11. Let $S_1 \cup \ldots \cup S_k$ be the maximum k-colorable subgraph with S_t stable sets. For every $t = 1, \ldots, k$, let $y^{(t)}$ be the vector defined by (51) for S_t. We may assume that S_t are pairwise disjoint. Then the vectors $y^{(t)}$ are pairwise orthogonal. The result follows by using the Fan's Theorem [44] (cf. (8)). □

COROLLARY 4.16 *If $\vartheta_k(G) < |V(G)|$ then $\chi(G) > k$.*

5 Routing problems

In this section we will mention a number of results relating eigenvalues of graphs (in particular $\lambda_2(G)$) to metric (distance) parameters and walks in graphs. A great variety of such results have been discovered recently. For example, eigenvalues are related to the diameter, mean distance, forwarding indices, routings, several properties of random walks on graphs, etc. We do not intend to be complete, so some parts will be covered with not too many details.

5.1 Diameter and the mean distance

There is a great interest in obtaining good upper bounds on the diameter of graphs. The diameter can be efficiently computed but in practice graphs with several hundreds of thousands of vertices are dealt with and eigenvalue bounds, which can sometimes be estimated "by construction" (analytically), come into play.

There is a lower bound

$$\operatorname{diam}(G) \geq \frac{4}{n\lambda_2(G)} \tag{52}$$

which was obtained by Brendan McKay (private communication, cf. [97] for a proof). More important is that there are upper bounds on the diameter of a graph G in terms of $\lambda_2(G)$ [97]:

$$\operatorname{diam}(G) \leq 2\left\lceil \sqrt{\frac{\lambda_n(G)}{\lambda_2(G)}}\sqrt{\frac{\alpha^2-1}{4\alpha}} + 1 \right\rceil \lceil \log_\alpha \frac{n}{2} \rceil \tag{53}$$

where α is any real number which is > 1. For any particular choice of n, λ_n, and λ_2 one can find the value of α which imposes the lowest upper bound on the diameter of the graph. See [97] for details. A good general choice is $\alpha = 7$.

In [97] another upper bound on the diameter of a graph is obtained

$$\operatorname{diam}(G) \leq 2\left\lceil \frac{\Delta + \lambda_2(G)}{4\lambda_2(G)} \ln(n-1) \right\rceil. \tag{54}$$

This improves a bound obtained previously by Alon and Milman [6], and usually also supersedes the bound obtained by F. Chung [28]. Another very

nice improvement was obtained by Chung, Faber, and Manteuffel [29]:

$$\mathrm{diam}(G) \le \left\lceil \frac{\cosh^{-1}(n-1)}{\cosh^{-1}\left((\lambda_n+\lambda_2)/(\lambda_n-\lambda_2)\right)} \right\rceil + 1\,. \tag{55}$$

where $\lambda_2 = \lambda_2(G)$ and $\lambda_n = \lambda_n(G)$.

A relation between the diameter and the spectral properties is also observed in [39]. Another diameter bound was obtained by Nilli [103]. If G contains two edges whose endvertices are at distance at least κ in G then

$$\lambda_2(G) \le \Delta - \sqrt{\Delta-1} + \frac{4\sqrt{\Delta-1}-2}{\kappa} \tag{56}$$

where Δ is the maximal vertex degree in the graph G. This bound holds also for weighted graphs, which is not the case with other bounds mentioned above. On the other hand, (56) makes sense only for the so-called *Ramanujan graphs* [89, 90] where $\lambda_2(G) \ge \Delta - \sqrt{\Delta-1}$.

In [97], some bounds on the mean distance $\bar{\rho}(G)$ are derived. Recall that the mean distance is equal to the average of all distances between distinct vertices of the graph. A lower bound is

$$(n-1)\bar{\rho}(G) \ge \frac{2}{\lambda_2(G)} + \frac{n-2}{2}$$

and an upper bound, similar to (54), is

$$\bar{\rho}(G) \le \frac{n}{n-1}\left\lceil \frac{\Delta+\lambda_2(G)}{4\lambda_2(G)}\ln(n-1)\right\rceil.$$

There is also an upper bound on $\bar{\rho}(G)$ related to the inequality (53). Cf. [97].

There is an interesting formula for the mean distance of a tree (due to B. D. McKay). See [92] or [97] for a proof.

THEOREM 5.1 *Let T be a tree of order n and $\lambda_2, \lambda_3, \ldots, \lambda_n$ the non-zero Laplacian eigenvalues of T. Then the mean distance $\bar{\rho}(T)$ is equal to:*

$$(n-1)\bar{\rho}(T) = 2\sum_{i=2}^{n}\frac{1}{\lambda_i}\,.$$

Some related results can also be found in [93].

5.2 Routings

Eigenvalues of graphs can also be used in relation to several problems which involve a system of shortest paths between vertices of a graph. Roughly speaking, one is interested in a set of shortest paths between all pairs of distinct vertices, $\mathcal{P} = \{P_{uv} \mid u, v \in V(G), u \neq v, P_{uv} \text{ is a geodesic path}\}$. Such a system of paths is called a *routing* on G. The goal is to find a routing which minimizes the maximal number of occurrences of any edge in the routing. There is also a vertex version of the problem. The obtained minimum is called the *forwarding index* (respectively, the *vertex forwarding index*) of the graph. There are some simple inequalities that relate the forwarding parameters with expanding properties of graphs, and these relations give rise to eigenvalue applications in these problems. We refer to [125] for details.

5.3 Random walks

It has been known for a long time that the properties of a random walk on a graph G and the spectral properties of its transition matrix $P(G)$ are closely related (see, e.g., [82]). Let us recall that the entries p_{uv} of the transition matrix are defined by $p_{uv} = a_{uv}/\deg(u)$, where a_{uv} is the element of the (weighted) adjacency matrix of G. We will only refer to some recent papers in this area. There is a close relationship between the random walk properties and combinatorial optimization, for example in the area of randomized algorithms. See, e.g., [87].

The *cover time* of a graph G is the maximum over all vertices $v \in V(G)$ of the expected time required in a random walk starting at v to visit all vertices of G. Results related to the cover time of graphs appear in [3, 20, 38, 39, 80, 109, 119]. A closely related notion is the *hitting time* of the random walk [2, 19, 107, 109].

The *mixing rate* of a random walk is a measure which measures how fast we approach the stationary distribution by starting the random walk at an arbitrary vertex. Related works are [1, 87, 124]. A random walk is *rapidly mixing* if it approaches stationary distribution "very fast" (in the logarithmic number of steps). For a random walk on a graph G this notion is closely related to $\lambda_2(G)$. Jerrum and Sinclair [70] obtained a fully polynomial approximation scheme for the permanent evaluation (and thus for counting the number of perfect matchings in graphs) by using the rapid mixing property.

Some other related results appeared in [4, 39, 107, 108, 128, 130].

6 Embedding problems

The eigenvalue approach is also useful in the study of embedding problems, where it is used to guarantee existence or nonexistence of certain graph embeddings. We include this topic in our survey, because determining the minimum dimension of an embedding has a flavour of an optimization problem. Moreover, the proofs rely on a different property of eigenvalues – on the Sylvester's law of inertia of symmetric quadratic forms.

Let G be a graph. The distance $\mathrm{dist}_G(u,v)$ of two vertices u and v is the length of a shortest path between u and v. The *distance* matrix $D = D(G)$ is the matrix of pairwise distances between the vertices of G.

A mapping $f : V(G) \to V(H)$ is called an *isometric embedding* of a graph G into a graph H if $\mathrm{dist}_H(f(u), f(v)) = \mathrm{dist}_G(u,v)$ for every pair $u, v \in V(G)$. A recent survey of results on isometric graph embedding problems can be found in [59]. We recall only two results, namely isometric embedding of graphs in cubes and squashed cubes, where eigenvalue technique was applied.

The *squashed cube* Q_r^* is the graph with vertex set $\{0,1,*\}^r$, and the edge set formed by the pairs $(u_1,\ldots,u_r)$ and $(v_1,\ldots,v_r)$ such that there is exactly one coordinate i for which $\{u_i, v_i\} = \{0,1\}$. P. Winkler [135] proved that every connected graph G can be isometrically embedded in a squashed cube Q_r^* of dimension $r \le |V(G)| - 1$. A lower bound on the minimum r was known earlier, and the result is reported to Witsenhausen (see [60]).

THEOREM 6.1 *Assume that a graph G can be isometrically embedded in the squashed cube Q_r^*. Then*

$$r \ge \max(n^+, n^-)$$

where n^+ and n^- denote the number of positive and negative eigenvalues of the distance matrix $D(G)$ of G.

PROOF. Let d_{ij} denote the distance $\mathrm{dist}_G(i,j)$. We will consider the quadratic form

$$\frac{1}{2}x^T D(G)x = \sum_{i<j} d_{ij}x_i x_j \tag{57}$$

in variables $x = (x_1,\ldots,x_n)^T$, $n = |V(G)|$.

Let $f : V(G) \to \{0,1,*\}^r$ be an isometric embedding of G in the squashed cube Q_r^*. For every $k = 1,\ldots,r$, let

$$X_k = \{i \mid f(i)_k = 0\} \quad \text{and} \quad Y_k = \{i \mid f(i)_k = 1\}\ .$$

The sets X_k, Y_k, $k = 1, \ldots, r$, are used to express the quadratic form (57) as

$$\sum_{i<j} d_{ij} x_i x_j = \sum_{k=1}^{r} \Big(\sum_{i \in X_k} x_i \Big) \Big(\sum_{j \in Y_k} x_j \Big) . \tag{58}$$

Using the identity $ab = \frac{1}{4}((a+b)^2 - (a-b)^2)$, this form can be written as a sum and difference of squares

$$\sum_{i<j} d_{ij} x_i x_j = \frac{1}{4} \sum_{k=1}^{r} \Big\{ \Big(\sum_{i \in X_k} x_i + \sum_{j \in Y_k} x_j \Big)^2 - \Big(\sum_{i \in X_k} x_i - \sum_{j \in Y_k} x_j \Big)^2 \Big\} . \tag{59}$$

By the Sylvester's law of inertia, the number of positive and negative squares must be at least n^+ and n^-, respectively. □

The *hypercube* Q_r is the graph with vertex set $\{0,1\}^r$, and two vertices $(u_1, \ldots, u_r)$ and $(v_1, \ldots, v_r)$ form an edge if $\sum_{i=1}^{r} |u_i - v_i| = 1$. The graphs G isometrically embeddable into a hypercube have been first characterized by Djoković [40]. From our point of view, the following characterization is interesting.

THEOREM 6.2 *([120]) A graph G is isometrically embeddable in a hypercube Q_r if and only if G is bipartite and the distance matrix $D(G)$ has exactly one positive eigenvalue.*

The dimension of the minimum embedding was determined by Graham and Pollack [60] as the number of negative eigenvalues of $D(G)$.

THEOREM 6.3 *([60]) Let a graph G be isometrically embeddable a hypercube Q_r. Then the minimum r (the dimension of the embedding) is equal to the number of negative eigenvalues of the distance matrix $D(G)$.* □

A Appendix: Computational aspects

In this Appendix we briefly discuss several ingredients of the computation and complexity of the problems arising by evaluating the eigenvalue bounds.

Complexity

The most commonly used model of complexity in the combinatorial optimization is the model based on the time complexity. From this point of view, problems are classified as 'easy' or 'difficult' depending on whether they are polynomial time solvable or NP-hard. A problem is said to be *polynomial time solvable*, if it admits a solution by an algorithm whose running time is bounded by a polynomial in the size of the input, measured by the length of the binary encoding. The opposite pole form the NP-hard problems, which are at least as difficult as the most difficult problems in the class NP (the class of nondeterministically polynomial problems). The formal definition of the complexity classes can be found in the book [53]. It is widely believed that the NP-complete problems cannot be solved in polynomial time, and the P=NP problem is definitely the most important open problem of the theoretical computer science.

There are only a few combinatorial optimization problems (like the graph isomorphism) whose complexity status is open. All the other most important problems are known to be either polynomial time solvable or NP-hard.

The combinatorial optimization problems surveyed in this article, with the exception of the edge- and vertex-connectivity studied in Section 2.2, belong to the NP-hard problems. Hence, the existence of good estimates is very important. Eigenvalue bounds provide in many cases quite good approximations. Moreover, as we show below, these estimates are efficiently computable.

Eigenvalue computation

Both in the direct formulas and the approximation by a continuous problem, we need to determine the eigenvalues numerically in order to get concrete bounds. The eigenvalues of a symmetric matrix are real but, in general, irrational numbers. Hence, given an integral (or rational) symmetric matrix M, we cannot compute its spectrum in polynomial time. However, it is known as a folklore result that the eigenvalues can be computed in polynomial time with an arbitrary prescribed precision. Unfortunately, we cannot refer to any detailed analysis of this question. Some partial discussions of this topic can be found in [8] and [36].

The polynomial time computability of eigenvalues has only theoretical importance. For applications, it is significant that the eigenvalues can be computed fast by a variety of numerical methods, see e.g., [58]. There also

exist several software packages [31, 123] for the eigenvalue computations. For example, the routine DNLASO from [123] was used by Poljak and Rendl [113] in the practical computations related to the max-cut problem.

Convexity

Convexity is a crucial property, which enables efficient solution of the relaxed continuous optimization problems.

Given a symmetric matrix M of size $n \times n$, an integer k, $1 \leq k \leq n$, and non-negative coefficients c_i, $i = k, k+1, \ldots, n$, satisfying $c_k \leq c_{k+1} \leq \cdots \leq c_n$, let us consider the function $f(u), u \in \boldsymbol{R}^n$, defined by

$$f(u) = \sum_{i=k}^{n} c_i \, \lambda_i(M + \mathrm{diag}(u)). \tag{60}$$

The following result is obtained by an easy application of the Rayleigh's principle (4) and the Fan's theorem (8).

THEOREM A.1 *[30] The function $f(u)$ defined by (60) is convex.* □

Hence the functions given by formulas (13), (14), (26), (35), and (36) are convex (resp. concave), and their minimum (resp. maximum) is efficiently computable, as mentioned in the next paragraph. It is also easy to see (by an application of the Rayleigh's principle) that the ϑ-function defined by (49) is obtained by the minimization of a convex function.

As a consequence of the convexity, dual characterizations are possible (cf. Theorems 2.11 and 4.12). A general duality theorem of that type is proved also in [105].

Global optimization

Another important fact is that the problem of the minimization of a convex function f over a convex region K in $\boldsymbol{R}^n$ is, under some technical assumptions on f and K, polynomial time solvable in the following sense. Given an $\varepsilon > 0$, the algorithm finds a rational number $\bar{z}$ and a rational vector $\bar{u} \in K$ such that $|\bar{z} - f(\bar{u})| \leq \varepsilon$, and

$$f(\bar{u}) \leq f(u) + \varepsilon \;\text{ for every } u \text{ such that } \; \{u' \in \boldsymbol{R}^n \mid \|u - u'\| < \varepsilon\} \subset K. \tag{61}$$

A detailed analysis of the ellipsoid algorithm for the minimization of f is given in the book by Grötschel, Lovász, and Schrijver [62].

The general theory can be applied to the convex function f given by (60) and the convex set $K = \{u \in \boldsymbol{R}^n \mid \sum_{i=1}^n u_i = 0\}$. In this concrete case, the minimum $\bar{u}$ can be approximated in a stronger sense, namely so that

$$f(\bar{u}) \leq f(u) + \varepsilon \quad \text{for all} \quad u \in K$$

holds (instead of (61)).

Again, the polynomial time computability is mainly of theoretical interest, because it indicates that the relaxed problems are easy. For the concrete computation, other algorithms than the ellipsoid method are more suitable. The problem of practical minimization of (60) is slightly complicated by the fact that f is not differentiable at all points. In particular, it is typically not differentiable at its minimum, because several eigenvalues are often identified as a result of the minimization.

Several methods of minimization of (60) were proposed in [30, 105, 122].

Branch and bound algorithms

The eigenvalue relaxations can also be used to compute exact optima in the combination with the branch and bound method. For that purpose, it is important to show that the relaxation is monotone with respect to the branching. Computational experiments for the max-cut problem were done by Poljak and Rendl [113]. In particular, the computing was speeded up by a suitable initiation of parameters in solving the subproblems. This was possible due to the combinatorial properties of the eigenvalue bound.

B Appendix: Eigenvalues of random graphs

The usual model for random graphs is the following. For a positive integer n we consider (labelled) graphs on n vertices in which each edge appears with probability $p = p(n)$. The adjacency matrix of a random graph is a random symmetric 01-matrix with zeros on the main diagonal. For a (random) graph G with the adjacency matrix A let us denote by $\overline{d}(A)$ the density of edges of G, more precisely, $\overline{d}(A) = 2|E(G)|/n^2$. The following bound is easy to verify:

PROPOSITION B.1 *([71]) Let G be a graph of order n and A its adjacency matrix. Then*

$$n\overline{d}(A) \leq \lambda_{\max}(A) \leq n\sqrt{\overline{d}(A)} \ .$$

PROOF. The first inequality follows by (1.5) by taking $x = \mathbf{1}$,

$$\lambda_{\max}(A) \geq \frac{(A\mathbf{1}, \mathbf{1})}{(\mathbf{1}, \mathbf{1})} = n\overline{d}(A) \ .$$

The other inequality follows from the fact that

$$\sum_{i=1}^{n} \lambda_i(A)^2 = tr\, A^2 = \sum_{v \in V(G)} deg(v) = n^2\overline{d}(A) \ .$$

□

Note that for random graphs the expected value of $\overline{d}(A)$ is $\frac{n-1}{n}p$ which is approximately equal to p. The bounds of Proposition B.1 hold in general. They can be improved for random graphs.

THEOREM B.2 *([71]) For almost all graphs of order n (with fixed edge probability p) the maximal eigenvalue of the adjacency matrix A is equal to*

$$\lambda_{\max}(A) = np(1 + o(1)) \, .$$

By the above result almost all graphs have the maximal eigenvalue close to np. This is to be expected. Much more surprising is the result for the second largest eigenvalue.

THEOREM B.3 *([71]) For almost all graphs G of order n with fixed edge probability p ($0 < p < 1$) and an arbitrary $\varepsilon > 0$, the second largest adjacency matrix eigenvalue is*

$$\lambda_{n-1}(A) = O(n^{1/2+\varepsilon}) \, .$$

These results were upgraded by Füredi and Komlós [52]:

THEOREM B.4 *([52]) Let $A = (a_{ij})$ be an $n \times n$ random symmetric matrix in which $a_{ii} = 0$ and a_{ij} $(i < j)$ are independent, identically distributed bounded random variables with distribution function H. Denote the moments of H by $\mu = \int x dH(x)$ and $\sigma^2 = \int (x - \mu)^2 dH(x)$. Then:*

(a) If $\mu > 0$ then $\lambda_{\max}(A) = \mu n + O(1)$ in measure, and $\max_{1 \leq i < n} |\lambda_i(A)| = 2\sigma\sqrt{n} + O(n^{1/3} \log n)$ in probability.

(b) If $\mu = 0$ then $\max_{1 \leq i \leq n} |\lambda_i(A)| = 2\sigma\sqrt{n} + O(n^{1/3} \log n)$ in probability.

□

The special case of Theorem B.4(a) where H is a discrete random variable with values 0 and 1, the latter with probability p, gives Theorem B.3. The additional step is a result of Wigner [131] which determines the overall eigenvalue distribution of random graphs.

THEOREM B.5 *([131]) Let $A = (a_{ij})$ be an $n \times n$ random symmetric matrix in which $a_{ii} = 0$ and a_{ij} $(i < j)$ are independent, identically distributed bounded random variables with distribution function H. Denote the moments of H by $\mu = \int x dH(x)$ and $\sigma^2 = \int (x-\mu)^2 dH(x)$, and let $F_n(x)$ be the cumulative distribution function of the eigenvalues of A. Then we have for an arbitrary x:*

$$\lim_{n\to\infty} F_n(x) = \int_{-\infty}^{x} f(x)\,dx \quad \textit{in probability}$$

where

$$f(x) = \begin{cases} \frac{1}{2\pi\sigma^2 n}\sqrt{4\sigma^2 n - x^2}, & |x| < 2\sigma\sqrt{n} \\ 0, & \textit{otherwise} \end{cases} .$$

□

It should be mentioned that Theorem C.4 does not follow from Theorem B.5. The latter result only implies that at most $o(n)$ eigenvalues are in absolute value larger than $2\sigma\sqrt{n}(1 + o(1))$. The non-symmetric random matrices were considered by Juhász [72].

The Laplacian spectrum of random graphs was considered by Juvan and Mohar [79]. (A weaker result was obtained independently by Juhász [74].) The distribution of eigenvalues follows easily from the Wigner's result (a version where the diagonal entries need not to be identically 0; cf. [71]). The important is the estimation of $\lambda_2(G)$ for a random graph G.

THEOREM B.6 *([79]) For a fixed edge probability p $(0 < p < 1)$ and any $\varepsilon > 0$ almost all graphs have their Laplace eigenvalues $\lambda_2(G)$ and $\lambda_{\max}(G)$ bounded by:*

$$pn - f_\varepsilon^+(n) < \lambda_2(G) < pn - f_\varepsilon^-(n)$$

and

$$pn + f_\varepsilon^+(n) > \lambda_{\max}(G) > pn + f_\varepsilon^-(n)$$

where

$$f_\varepsilon^+(n) = \sqrt{(2+\varepsilon)p(1-p)n\log n} \quad \textit{and} \quad f_\varepsilon^-(n) = \sqrt{(2-\varepsilon)p(1-p)n\log n}.$$

□

There were also serious attacks on the eigenvalue problem for random regular graphs. For an integer $d \geq 2$ consider random d-regular graphs. McKay [91] determined the expected eigenvalue distribution of large d-regular graphs. Moreover, his result approximates eigenvalue distribution for arbitrary large regular graphs which do not have too many short cycles (which is the case with random regular graphs in any sensible model).

THEOREM B.7 *([91]) Let $d \geq 2$ be a fixed integer and let $G_1, G_2, G_3, \ldots$ be a sequence of simple d-regular graphs with increasing orders and such that for each $k \geq 3$ the number $c_k(G_n)$ of cycles of length k in G_n satisfies*

$$\lim_{n\to\infty} c_k(G_n)/|V(G_n)| = 0 \ .$$

Then the cumulative eigenvalue distribution functions $F(G_n, x)$ of graphs G_n converge to $F(x)$ for every x, where $F(x) = \int_{-\infty}^{x} f(t)dt$ and

$$f(t) = \begin{cases} \frac{d\sqrt{4(d-1)-t^2}}{2\pi(d^2-t^2)}, & |t| \leq 2\sqrt{d-1} \\ 0, & otherwise \end{cases} \ .$$

□

Godsil and Mohar [56] determined the expected eigenvalue distribution of random semiregular bipartite graphs (and some other families). Recall that a bipartite graph G is (d_1, d_2)-*semiregular* if the vertices in one bipartition class all have degree d_1, and the vertices in the other class have degree d_2.

THEOREM B.8 *([56]) Let $d_1, d_2 \geq 2$ be a integers, $p = \sqrt{(d_1-1)(d_2-1)}$, and let $G_1, G_2, G_3, \ldots$ be a sequence of simple (d_1, d_2)-semiregular bipartite graphs with increasing orders and such that for each $k \geq 3$ the number $c_k(G_n)$ of cycles of length k in G_n satisfies*

$$\lim_{n\to\infty} c_k(G_n)/|V(G_n)| = 0 \ .$$

Then the cumulative eigenvalue distribution functions $F(G_n, x)$ of graphs G_n converge to $F(x)$ for every x, where

$$F(x) = \int_{-\infty}^{x} f(t)dt + \frac{1}{2}\frac{|d_1 - d_2|}{d_1 + d_2}\delta(0)$$

where $\delta(0)$ is the discrete distribution with a unit point mass at the point 0, and

$$f(t) = \begin{cases} \dfrac{d_1 d_2 \sqrt{-(t^2 - d_1 d_2 + (p-1)^2)(t^2 - d_1 d_2 + (p+1)^2)}}{\pi(d_1 + d_2)(d_1 d_2 - t^2)|t|}, \\ \qquad \textit{if } |\sqrt{d_1 - 1} - \sqrt{d_2 - 1}| \le |t| \le \sqrt{d_1 - 1} + \sqrt{d_2 - 1} \\ 0, \qquad \textit{otherwise .} \end{cases}$$

□

The above result shows that all but $o(n)$ eigenvalues of a random d-regular graph are in absolute value smaller than $2\sqrt{d-1}$. However, due to the importance of the second eigenvalue of graphs, this is not a sufficient result for applications surveyed in this paper. Broder and Shamir [21] were able to show that random d-regular graphs (for d an even integer) have

$$\rho_2(G) = O(d^{3/4})$$

where

$$\rho_2(G) = \max\{|\lambda| \,;\ \lambda \text{ an eigenvalue of } A(G), \lambda \neq d\} \ .$$

The above estimate holds for almost all d-regular graphs according to the following model. Let d be an even integer. For a random d-regular graph on n vertices choose $\frac{d}{2}$ random permutations $\sigma_1, \sigma_2, \ldots, \sigma_{d/2}$ of $V = \{1, 2, \ldots, n\}$, and define the d-regular graph corresponding to these permutations as the graph on the vertex set V with the vertex i $(1 \le i \le n)$ adjacent to vertices $\sigma_j(i), \sigma_j^{-1}(i)$, $j = 1, 2, \ldots, \frac{d}{2}$. (Note that some of the obtained graphs contain loops or parallel edges. If we do not want loops we may consider random fixed point free permutations σ_j. It turns out, however, that a positive portion of these graphs are simple, so the properties holding for almost all graphs in this model also hold for almost all simple graphs among them.)

The $O(d^{3/4})$ bound for $\rho_2(G)$ was improved to $O(\sqrt{d})$ by Friedman (using the same model) [50]. A weaker version than Friedman's was obtained independently by Kahn and Szemerédi (cf. [51]). They proved the following results:

THEOREM B.9 *([51]) For a fixed even integer d, a random d-regular graph G of order n has*

$$\rho_2(G) = O(\sqrt{d})$$

with probability $1 - n^{-\Omega(\sqrt{d})}$ as n tends to infinity. □

It is not known if the methods used by Kahn and Szemerédi yield the expected bound $(2+o(1))\sqrt{d-1}$ with probability $1-o(1)$.

THEOREM B.10 *([50]) For a fixed even integer d, a random d-regular graph G of order n has the expectation*

$$E(\rho_2(G)^m) \le \left(2\sqrt{d-1} + 2\log d + O(1) + O\Big(\frac{d^{3/2}\log\log n}{\log n}\Big)\right)^m$$

for any integer $m \le 2\lfloor \log n \lfloor \sqrt{d-1}/2 \rfloor / \log(d/2) \rfloor$ (with an absolute constant in the O-notation), where all logarithms are base e. □

The following result is even more useful:

THEOREM B.11 *([50]) For a fixed even integer d and an arbitrary $\varepsilon > 0$, a random d-regular graph G of order n has*

$$\rho_2(G) \le \left(2\sqrt{d-1} + 2\log d + O(1) + O\Big(\frac{d^{3/2}\log\log n}{\log n}\Big)\right)(1+\varepsilon)$$

with probability at least $1-(1+\varepsilon)^2 n^{-2\lfloor\sqrt{d-1}/2\rfloor \log(1+\varepsilon)/\log(d/2)}$. □

On the other hand, Alon and Boppana (cf. [5]) proved that

$$\rho_2(G) \ge 2\sqrt{d-1} - O\Big(\frac{\log d}{\log n}\Big)$$

hold for any d-regular graph G, as far as $n \ge d^2$. Friedman's results are close to this bound but still far from the bound $\rho_2(G) \le 2\sqrt{d-1}+\varepsilon$ conjectured for random d-regular graphs by Alon [5].

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