

A spectral approach to bandwidth and separator problems in graphs

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Abstract

Lower bounds on the bandwidth, the size of a vertex separator of general undirected graphs, and the largest common subgraph of two undirected (weighted) graphs are obtained. The bounds are based on a projection technique developed for the quadratic assignment problem, and once more demonstrate the importance of the extreme eigenvalues of the Laplacian. They will be shown to be strict for certain classes of graphs and compare favourably to bounds already known in literature. Further improvement is gained by applying nonlinear optimization methods.

Keywords: bandwidth, vertex separator, Laplacian eigenvalues

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1 Introduction

The bandwidth of a graph is a graph invariant that is computationally extremely difficult to determine. A survey on the bandwidth of graphs and related problems is contained in e.g. [2]. Heuristics to find good labelings of vertices of graphs were developed by engineers as early as in the 60's to facilitate Finite Element calculations of structural design problems, see e.g. [17]. To estimate how close these labelings come to the minimal bandwidth, it is important to have good lower bounds on the minimal bandwidth. Recently, spectral properties of graphs were used to bound the bandwidth from below, see e.g [10, 11].

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In the present paper we strengthen the approach described in [10, 11] and derive new lower bounds for graph invariants related to the bandwidth. In particular, we get bounds on the size of balanced vertex separators in graphs.

The paper is organized as follows. In Section 2 we derive the mathematical tools necessary to obtain the new bounds. These tools are applied in Section 3 to the bandwidth problem, and in Section 4 to the vertex separator problem. In particular, we present two bounds on the bandwidth problem. The first bound, given in Theorem 8, uses only two extreme eigenvalues of the Laplacian matrix. The second bound, given in Theorem 9, is in the form of an efficiently solvable convex optimization problem, and makes use of the whole Laplacian spectrum. In Section 5 we shortly discuss the problem of finding the largest common subgraph of two given graphs whose special cases can also be applied to get some information on the bandwidth problem. Section 6 contains applications of our approach to the closely related 1-sum problem. We show that our new bound improves an earlier bound by Juvan and Mohar [10]. We close with some computational experiments in Section 7.

2 The tools

Let G be an undirected weighted graph having (weighted) adjacency matrix A . For $S_1, S_2 \subseteq V(G)$ denote by

$$\text{cut}(S_1, S_2) := \sum_{i \in S_1, j \in S_2} a_{ij}$$

the total weight of edges between the sets S_1 and S_2 . Lower bounds on $\text{cut}(S_1, S_2)$ for all (disjoint) sets S_1, S_2 of specified cardinalities $|S_i| = m_i$ ($i = 1, 2$) play a fundamental role in the analysis of several graph problems, like bounding the bandwidth, or finding vertex separators. The following theorem provides a lower bound on $\text{cut}(S_1, S_2)$ in terms of m_1, m_2 and the extreme Laplacian eigenvalues of G . The approach is based on partitioning results from [16]. Given numbers n, λ_2 , and λ_n define the following symmetric function on positive integers t_1, t_2 smaller than n :

$$f(t_1, t_2) := \frac{\sqrt{t_1 t_2}}{2n} \left[\left(\sqrt{t_1 t_2} + \sqrt{(n-t_1)(n-t_2)} \right) \lambda_2 + \left(\sqrt{t_1 t_2} - \sqrt{(n-t_1)(n-t_2)} \right) \lambda_n \right] \quad (1)$$

Theorem 1 *Let G be an undirected graph of order n . Let λ_2 and λ_n denote the second smallest and the largest Laplacian eigenvalue of G , respectively. If m_1, m_2, m_3 are positive integers summing up to n , then*

$$\text{cut}(S_1, S_2) \geq f(m_1, m_2)$$

for all partitions (S_1, S_2, S_3) of $V(G)$ into subsets of cardinalities $|S_i| = m_i$, $i = 1, 2, 3$.

Before proving this theorem, we need some auxiliary results. Following [16], we represent a partition (S_1, S_2, S_3) of $V(G)$ by an associated $n \times 3$ matrix X , where

$$x_{ij} = \begin{cases} 1 & \text{if } i \in S_j \\ 0 & \text{if } i \notin S_j. \end{cases}$$

The columns of X will be denoted by x_1, x_2, x_3 . Let

$$B = \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}.$$

It is easy to see that $\text{tr } X^t A X B = x_1^t A x_2 + x_2^t A x_1$ which in turn implies that

$$\text{cut}(S_1, S_2) = \frac{1}{2} \text{tr } X^t A X B. \quad (2)$$

In [16] it is shown that X describes a partition of $V(G)$ into subsets of specified sizes $m = (m_1, m_2, m_3)^t$ if and only if

$$X^t u_n = m, \quad X u_3 = u_n, \quad (3)$$

$$X^t X = M, \quad (4)$$

$$X \geq 0 \text{ elementwise.} \quad (5)$$

Throughout the paper we will denote by u , (or u_n to indicate the size) a vector of all ones, I_n the identity matrix of order n , $M := \text{diag}(m)$, and V will be an $n \times (n-1)$ matrix satisfying:

$$V^t V = I_{n-1}, \quad V^t u_n = 0. \quad (6)$$

The eigenvalues of a symmetric matrix Q of order n will be denoted by $\lambda_1(Q) \leq \dots \leq \lambda_n(Q)$. Finally, let $\bar{m} := (\sqrt{m_1}, \sqrt{m_2}, \sqrt{m_3})^t$, and let W be a 3×2 matrix satisfying:

$$W^t W = I_2, \quad W^t \bar{m} = 0.$$

Then

$$W W^t = I_3 - \frac{1}{n} \bar{m} \bar{m}^t. \quad (7)$$

The following result was proved in [16].

Proposition 2 *A matrix X satisfies (3), (4) if and only if there exists an $(n-1) \times 2$ matrix Z with $Z^t Z = I_2$ such that*

$$X = \frac{1}{n} u_n u_3^t M + V Z W^t M^{1/2}.$$

It is also easy to see that

$$\text{tr } X^t (A + D) X B = \text{tr } X^t A X B \quad (8)$$

for all diagonal matrices D , and all matrices X representing partitions. Let $s(A) := u^t A u$, and $r(A) := A u$. The following choice of D will turn out to be particularly useful:

$$D := \frac{s(A)}{n} I_n - \text{diag}(r(A)). \quad (9)$$

Note that $\text{tr } D = 0$. To prove Theorem 1 we need to know the eigenvalues of the 2×2 matrix

$$\tilde{M} := \sqrt{m_1 m_2} W^t B W.$$

Lemma 3 *The eigenvalues $\mu_1 \geq \mu_2$ of the matrix \tilde{M} are given by*

$$\mu_{1,2} = \frac{1}{n} \left(-m_1 m_2 \pm \sqrt{m_1 m_2 (n - m_1)(n - m_2)} \right).$$

Proof. We observe that μ_1 and μ_2 are characterized by

$$\begin{aligned} \mu_1 + \mu_2 &= \text{tr } \tilde{M} = -\frac{2m_1 m_2}{n}, \\ \mu_1^2 + \mu_2^2 &= \text{tr } \tilde{M}^2 = \frac{2m_1 m_2}{n} \left(m_3 + \frac{2m_1 m_2}{n} \right). \end{aligned}$$

After substituting the given values for μ_1 and μ_2 , the lemma follows. \square

We point out that

$$f(m_1, m_2) = -\frac{1}{2}\mu_2\lambda_2 - \frac{1}{2}\mu_1\lambda_n. \quad (10)$$

Next we relate the eigenvalues of

$$\tilde{A} := V^t(A + D)V$$

to the Laplacian eigenvalues of G . Let $\lambda_1 \leq \dots \leq \lambda_n$ denote the eigenvalues of the Laplacian $L := \text{diag}(r(A)) - A$ of our weighted graph G .

Lemma 4 *The eigenvalues of the matrix $V^t(A + D)V$ are*

$$\nu_i = \frac{s(A)}{n} - \lambda_i, \quad i = 2, 3, \dots, n.$$

Proof. First note that $V^t(A + D)V = V^t\left(\frac{s(A)}{n}I - L\right)V$. Let x be an eigenvector for λ_i , where $i > 1$. Then $x \perp u$, since u is eigenvector of λ_1 . By (6), there exists a nonzero vector y such that $x = Vy$. We conclude that

$$\begin{aligned} V^t(A + D)Vy &= \frac{s(A)}{n}y - V^tL(Vy) \\ &= \frac{s(A)}{n}y - V^t(\lambda_i Vy) \\ &= \left(\frac{s(A)}{n} - \lambda_i\right)y. \end{aligned}$$

\square

We will also make use of the following two variations of the Hoffman–Wielandt inequality. We formulate these results as optimization problems, where the optimal objective function value is given by the eigenvalues of the underlying matrices. These results were first used to get tractable relaxations of graph partition problems and quadratic assignment problems.

Theorem 5 *Let A and B be symmetric matrices of order n and k , respectively, and suppose that $k \leq n$. Then*

$$\min\{\text{tr } AXBX^t : X^tX = I_k\} = \min\left\{\sum_{i=1}^k \lambda_i(B)\lambda_{\phi(i)}(A) : \phi \text{ injection}\right\}.$$

Proof. A similar result has been shown in [12] and is also implicitly contained in e.g. [6], where the theorem is proved for the case $k = n$, and both matrices positive definite. The proof easily generalizes to the present situation. For the sake of completeness we include the following argument and note that a similar result is also proved in [14].

We use the spectral decompositions of A and B ,

$$A = PEP^t, \quad B = QFQ^t,$$

with orthogonal matrices P, Q and diagonal matrices E, F of appropriate sizes. Note that the matrix $Y := P^t X Q$ has orthonormal columns, so we get:

$$\operatorname{tr} AXBX^t = \operatorname{tr} EYFY^t \tag{11}$$

$$= \sum_{i=1}^n \sum_{j=1}^k \lambda_i(A) \lambda_j(B) y_{ij}^2 \tag{12}$$

$$\geq \min \left\{ \sum_{i,j} \lambda_i(A) \lambda_j(B) z_{ij} : \sum_i z_{ij} = 1, \sum_j z_{ij} \leq 1, z_{ij} \geq 0 \right\} \tag{13}$$

$$= \min \left\{ \sum_{i=1}^k \lambda_i(B) \lambda_{\phi(i)}(A) : \phi \text{ injective} \right\}. \tag{14}$$

The last equality follows from the fact that the transportation constraints on the z_{ij} are totally unimodular. Therefore there exists an optimal 0-1 solution to the minimization problem, and these are characterized by injections $\phi : \{1, \dots, k\} \rightarrow \{1, \dots, n\}$.

To see that equality holds, it is sufficient to take an ordering of the eigenvalues and eigenvectors in E, F, P and Q given by the minimal injection and using $X = PQ^t$ to get attainment for the lower bound. In particular, P contains only the eigenvectors corresponding to the k eigenvalues of the image of ϕ in the ‘‘correct’’ ordering. \square

In the subsequent theorem we use the following sets of matrices: The set $\mathcal{O} := \{X : X^t X = I_n\}$ contains orthogonal matrices, and $\mathcal{E} := \{X : Xu = X^t u = u\}$ contains all matrices with row and column sums equal to one. Finally, the set of permutation matrices is denoted by Π .

Theorem 6 [8]. *Let A and B be symmetric matrices of order n , and suppose that $Au = \alpha u$. Then*

$$\begin{aligned} \max\{\operatorname{tr} AXBX^t : X \in \Pi\} &\leq \max\{\operatorname{tr} AXBX^t : X \in \mathcal{O} \cap \mathcal{E}\} \\ &= \sum_{i=1}^{n-1} \lambda_i(V^t AV) \lambda_i(V^t BV) + \frac{\alpha s(B)}{n}. \end{aligned} \tag{15}$$

We are now ready to prove Theorem 1.

Proof of Theorem 1. Using equalities (2), (9), and (8), and the characterization (3), (4), (5) for partitions X , we conclude that

$$\operatorname{cut}(S_1, S_2) \geq \min \left\{ \frac{1}{2} \operatorname{tr} X^t (A + D) X B : X \text{ satisfies (3), (4)} \right\} =: g(m_1, m_2) \tag{16}$$

for all partitions (S_1, S_2, S_3) with subsets of specified sizes m_1, m_2, m_3 . We will show that $g(m_1, m_2) = f(m_1, m_2)$. Substituting the parametrization of X from Proposition 2 we obtain after some rearrangement of terms

$$g(m_1, m_2) = \min \left\{ \frac{m_1 m_2 s(A)}{n^2} + \frac{1}{2} \operatorname{tr} \tilde{A} Z \tilde{M} Z^t : Z^t Z = I_2 \right\}.$$

We note in particular that due to the special choice of D we have

$$V^t(A + D)u = 0.$$

Therefore the terms linear in Z vanish. The minimum is given by Theorem 5. By Lemma 3, $\mu_2 \leq 0 \leq \mu_1$. Thus, using Theorem 6 we get

$$\min\{\operatorname{tr} \tilde{A} Z \tilde{M} Z^t : Z^t Z = I_2\} = \mu_2 \lambda_{\max}(\tilde{A}) + \mu_1 \lambda_{\min}(\tilde{A}).$$

A simple calculation using the spectral information from Lemma 4 shows that the terms containing $s(A)$ cancel, leaving the sum (10) of products of eigenvalues. \square

In the sequel, Theorem 6 will be applied several times in situations when one of the matrices A or B is the Laplacian matrix L of a (weighted) graph. In such cases, expression (15) becomes particularly simple, since the spectrum of $V^t L V$ consists of the eigenvalues of L but the eigenvalue zero. Let us recall that the Laplacian matrix $L = L(G)$ of a (weighted) graph G is defined by $L(G) = \operatorname{diag}(r(A)) - A$ where A is the (weighted) adjacency matrix of G , and $r(A)$ is the vector of the row sums of A . The following lemma follows easily from the proof of Lemma 4.

Lemma 7 *The Laplacian matrix $L(G)$ has the following properties.*

- (i) *If the edge weights of G are nonnegative, then $L(G)$ is positive semidefinite.*
- (ii) *$u = (1, \dots, 1)^t$ is an eigenvector of $L(G)$ corresponding to the eigenvalue 0.*
- (iii) *The spectrum of $V^t L(G) V$ (where V is the projection matrix satisfying (6)) consists of the eigenvalues of L where the multiplicity of the eigenvalue zero is decreased by one.*

\square

3 Bounding the bandwidth

The *bandwidth* $\sigma_\infty(G)$ of an n -vertex graph G is defined as

$$\sigma_\infty(G) := \min \left\{ \max_{ij \in E} |\phi(i) - \phi(j)| : \phi \text{ bijection } V(G) \rightarrow \{1, \dots, n\} \right\}. \quad (17)$$

Determining $\sigma_\infty(G)$ is computationally an extremely difficult task. Several lower bounds on $\sigma_\infty(G)$ expressed in terms of the Laplacian eigenvalues of G are obtained in [10] and further

developed and improved in [11]. A basic proof technique to derive lower bounds on $\sigma_\infty(G)$ consists in showing that

$$\text{cut}(S_1, S_2) > 0$$

for all S_1, S_2 with $|S_1| = m_1 > 0, |S_2| = m_2 > 0$. If this is the case, it follows that

$$\sigma_\infty(G) \geq (n - m_1 - m_2) + 1, \tag{18}$$

because using a bijection ϕ where the minimum in (17) is attained, there are edges between $S_1 := \{\phi^{-1}(1), \dots, \phi^{-1}(m_1)\}$ and $S_2 := \{\phi^{-1}(n - m_2 + 1), \dots, \phi^{-1}(n)\}$. Using Theorem 1, we obtain the following lower bound on $\sigma_\infty(G)$.

Theorem 8 *Let G be an undirected graph on n vertices with at least one edge. Let λ_2 and λ_n denote the second smallest and the largest Laplacian eigenvalue of G , respectively. Let α be the largest integer smaller than $n\lambda_2/\lambda_n$.*

- (a) *If $\alpha \geq n - 2$, then $G = K_n$ and $\sigma_\infty(G) = n - 1$.*
- (b) *If $\alpha \leq n - 2$ and $n - \alpha = 0 \pmod{2}$, then $\sigma_\infty(G) \geq \alpha + 1$.*
- (c) *Otherwise $\sigma_\infty(G) \geq \alpha$.*

Proof. To prove (a) we note that we can set $m_1 = m_2 = 1$ to get

$$\text{cut}(S_1, S_2) \geq f(1, 1) = \frac{\lambda_n}{2n} \left(\frac{n\lambda_2}{\lambda_n} - (n - 2) \right) > 0$$

and therefore the bandwidth is $n - 1$, so G is the complete graph.

In case (b) we first note that in the special case $\alpha = 0$ the theorem is trivially true because G contains edges. Therefore consider $n - 2 \geq \alpha > 0$ and $n - \alpha = 2s > 0$. Applying Theorem 1 with $m_1 = m_2 = s > 0$ and $m_3 = \alpha > 0$ we obtain

$$\text{cut}(S_1, S_2) \geq f(s, s) = \frac{s\lambda_n}{2n} \left(\frac{n\lambda_2}{\lambda_n} - \alpha \right) > 0.$$

Therefore $\sigma_\infty(G) \geq \alpha + 1$.

Finally suppose $n - \alpha = 2s + 1$ and $s > 0$. We set $m_1 = m_2 = s + 1$ and $m_3 = \alpha - 1$ to show similarly that in this case $\sigma_\infty(G) \geq \alpha$. □

We note that (c) could be improved slightly by testing whether $f(s + 1, s) > 0$ in which case $\sigma_\infty(G) \geq \alpha + 1$.

An alternate way to derive bounds on the bandwidth consists in using the *Quadratic Assignment Problem* (QAP) as a relaxation. The QAP consists in optimizing

$$\text{tr} AXBX^t$$

over the set Π of permutation matrices X . We assume that the matrices A and B , defining QAP, are symmetric.

As before, we denote by L the Laplacian matrix of a given graph G . Although G is unweighted, we may assign arbitrary weights to its edges, and then let L be the weighted Laplacian. To test whether $\sigma_\infty(G) > k$, we define the following set of $n \times n$ matrices:

$$\mathcal{B}_k := \{B : B = B^t, b_{ij} = 0 \text{ if } |i - j| \leq k\}.$$

Theorem 9 *Let L denote an arbitrary weighted Laplacian matrix of a graph G . If there exists a matrix $B \in \mathcal{B}_k$ such that*

$$\sum_{i=1}^{n-1} \lambda_{i+1}(L) \lambda_i(V^t B V) < 0, \quad (19)$$

then $\sigma_\infty(G) > k$.

Proof. Suppose that $\sigma_\infty(G) \leq k$ and let $B \in \mathcal{B}_k$ be arbitrary. Let the vertices of G be labeled such that $b_{ij} = 0$ whenever $|i - j| > k$. Then we can apply Theorem 6 to the matrices L and B , since $\alpha = 0$ is eigenvalue of L for the eigenvector u . Using Lemma 7 (iii) we get

$$0 = \text{tr } LB \leq \max\{\text{tr } LXB X^t : X \in \mathcal{O} \cap \mathcal{E}\} = \sum_{i=1}^{n-1} \lambda_{i+1}(L) \lambda_i(V^t B V).$$

This shows that (19) is not possible. □

Consider the following matrix

$$\hat{B} = \begin{pmatrix} \mathbf{0}_{m_1 \times m_1} & \mathbf{0}_{m_1 \times m_3} & \mathbf{1}_{m_1 \times m_2} \\ \mathbf{0}_{m_3 \times m_1} & \mathbf{0}_{m_3 \times m_3} & \mathbf{0}_{m_3 \times m_2} \\ \mathbf{1}_{m_2 \times m_1} & \mathbf{0}_{m_2 \times m_3} & \mathbf{0}_{m_2 \times m_2} \end{pmatrix}$$

where $\mathbf{0}_{i \times j}$ and $\mathbf{1}_{i \times j}$ denotes the $i \times j$ matrix of all zeros and all ones, respectively. Obviously, $\hat{B} \in \mathcal{B}_{m_3}$. Using an argument similar to the proof of Lemma 3, one easily finds that the nonzero eigenvalues of the matrix $V^t \hat{B} V$ are equal to μ_1 and μ_2 as given by Lemma 3. Therefore, we conclude that

$$\min_{B \in \mathcal{B}_{m_3}} \text{QAP}(L, B) \leq \text{QAP}(L, \hat{B}) = \mu_2 \lambda_2 + \mu_1 \lambda_n = -2f(m_1, m_2),$$

where the last equation is just (10). This shows that the bound given by Theorem 8 is contained in Theorem 9.

We conclude with another application of the Quadratic Assignment model to derive an upper bound on the bandwidth.

Let G be a nonempty graph of order n with m edges. Let $A = (a_{ij})$ denote the adjacency matrix of G , and let $B = (b_{ij})$ be an $n \times n$ symmetric matrix defined by $b_{ij} = m^{|i-j|-1}$ for $i \neq j$ and $b_{ii} = 0$. Let

$$\text{QAP}(A, B) := \max_{\pi} \sum_{i,j} a_{ij} b_{\pi(i)\pi(j)}$$

denote the value of the optimum solution of the quadratic assignment problem with matrices A and B . We have the following result.

Proposition 10 *The bandwidth of G is at most k if and only if $\text{QAP}(A, B) \leq 2m^k$. Hence,*

$$\sigma_\infty(G) = \left\lceil \log_m \frac{1}{2} \text{QAP}(A, B) \right\rceil \leq \left\lceil \log_m \frac{1}{2} \sum_{i=1}^{n-1} \lambda_{i+1}(L(G)) \lambda_i(-V^t B V) \right\rceil.$$

Proof. The statement is obvious for $m = 1$. Hence we will assume that G has at least two edges. Assume that the bandwidth is at most k . Then there exists a permutation π such that $|\pi(i) - \pi(j)| \leq k$ for all edges ij . Thus, $a_{ij} b_{\pi(i)\pi(j)} \leq m^{k-1}$ for every pair i, j , and $\sum_{i,j} a_{ij} b_{\pi(i)\pi(j)} \leq 2m \cdot m^{k-1} = 2m^k$. Conversely, assume that $\sigma_\infty(G) > k$. Then, for every permutation π , there exists an edge $i_0 j_0$ such that $|\pi(i_0) - \pi(j_0)| > k$, i.e. $a_{i_0 j_0} b_{\pi(i_0)\pi(j_0)} \geq m^k$. Since $m > 1$, we conclude that $\sum_{i,j} a_{ij} b_{\pi(i)\pi(j)} > 2m^k$. This proves the first statement. As an immediate consequence we get $\sigma_\infty(G) = \left\lceil \log_m \frac{1}{2} \text{QAP}(A, B) \right\rceil$. We will estimate $\text{QAP}(A, B)$ as follows. Let $L = L(G)$ denote the Laplacian matrix of G . Since the diagonal entries of B are zero, we have $\text{QAP}(A, B) = \text{QAP}(-L, B)$. By Lemma 7 (iii), the eigenvalues of $V^t L V$ are $\lambda_2, \dots, \lambda_n$. Since $Lu = 0 \cdot u$, applying Theorem 6 (with $\alpha = 0$) yields the upper bound

$$\text{QAP}(-L, B) = \max\{\text{tr } A X B X^t : X \in \Pi\} \leq \sum_{i=1}^{n-1} \lambda_{n-i+1}(L(G)) \lambda_i(V^t B V).$$

□

4 Lower Bounds on Vertex Separators

A *vertex separator* $S \subset V$ partitions the vertices of a graph G into three sets S_1, S_2 and $S_3 = S$ such that no vertex of S_1 is adjacent to a vertex of S_2 . In applications S_3 should be a small set separating two large sets of roughly the same size. Here, S_3 is called a *balanced separator* if $2|S_1| \geq |S_2|$ and $2|S_2| \geq |S_1|$. By means of Theorem 1 we shall derive a new lower bound on the cardinality of such separators.

Suppose S_3 separates S_1 and S_2 and let $m_1 = |S_1|$ and $m_2 = |S_2|$. Then $\text{cut}(S_1, S_2) = 0$, and Theorem 1 yields a lower bound on $|S_3|$.

Theorem 11 *Let G be a graph on n vertices. Let λ_2 and λ_n denote the second smallest and the largest Laplacian eigenvalue of G , respectively. If $S_3 \subset V$ separates vertex sets S_1, S_2 then*

$$|S_3| \geq \frac{4\lambda_n \lambda_2 |S_1| |S_2|}{n(\lambda_n - \lambda_2)^2}. \quad (20)$$

Proof. Let $m_i = |S_i|$ for $i \in \{1, 2, 3\}$ and suppose S_3 separates S_1 and S_2 . By Theorem 1, $0 = \text{cut}(S_1, S_2) \geq f(m_1, m_2)$. Therefore we conclude:

$$(m_1 + m_3)(m_2 + m_3)(\lambda_n - \lambda_2)^2 \geq m_1 m_2 (\lambda_n + \lambda_2)^2$$

or equivalently

$$n m_3 \geq \frac{m_1 m_2 ((\lambda_n + \lambda_2)^2 - (\lambda_n - \lambda_2)^2)}{(\lambda_n - \lambda_2)^2},$$

and (20) follows immediately. \square

For a discussion of the tightness of this bound we shall need the following binary graph operations. Let G_1 and G_2 be unweighted vertex disjoint graphs. Denote by $G_1 \cup G_2$ their *union*, and let $G_1 * G_2$ be their *join* (obtained from $G_1 \cup G_2$ by joining every vertex of G_1 with every vertex of G_2). The characteristic polynomial $\varphi(G, \lambda) = \prod_{i=1}^n (\lambda - \lambda_i(A(G)))$ of the resulting graph G can be expressed in terms of the characteristic polynomials of G_1 and G_2 . With $n = n_1 + n_2$,

$$\begin{aligned}\varphi(G_1 \cup G_2, \lambda) &= \varphi(G_1, \lambda) \varphi(G_2, \lambda), \\ \varphi(G_1 * G_2, \lambda) &= \frac{\lambda(\lambda - n)}{(\lambda - n_1)(\lambda - n_2)} \varphi(G_1, \lambda - n_2) \varphi(G_2, \lambda - n_1).\end{aligned}$$

Consider the class of graphs of the form $G = (G_1 \cup G_2) * G_3$ where the G_i are graphs of orders m_1, m_2, m_3 , respectively. The smallest possible separator is of size m_3 provided $m_3 \leq m_1 + m_2$. By the above formulas, if $m_3 \leq m_1 + m_2$, then $\lambda_n(G) = n = m_1 + m_2 + m_3$ and $\lambda_2(G) = m_3$. Thus, (20) is tight whenever $m_1 = m_2$.

To deduce a lower bound for balanced separators from (20), we parameterize m_1 and m_2 by $m_1 = t(n - m_3)$ and $m_2 = (1 - t)(n - m_3)$ for $t \in [\frac{1}{3}, \frac{2}{3}]$. The minimum of the right hand side of (20) with respect to t is obtained for $t \in \{\frac{1}{3}, \frac{2}{3}\}$. For balanced separators the bound now reads ($m_3 = |S_3|$):

$$m_3 \geq \frac{8}{9} \frac{\lambda_n \lambda_2}{(\lambda_n - \lambda_2)^2} \frac{(n - m_3)^2}{n}.$$

By solving the quadratic equation for m_3 , we get the following:

Corollary 12 *Let G be a graph on n vertices. Let λ_2 and λ_n denote the second smallest and the largest Laplacian eigenvalue of G , respectively. If $S_3 \subset V$ is a balanced vertex separator of G , then*

$$m_3 \geq n \left(1 + \frac{9}{16} \mu(G) - \sqrt{\left(1 + \frac{9}{16} \mu(G) \right)^2 - 1} \right)$$

where

$$\mu(G) = \frac{(\lambda_n - \lambda_2)^2}{\lambda_n \lambda_2}.$$

If the graph G is connected, the lower bounds derived above are closely related to the condition number $\text{cond}_2(V^t L V)$ of the matrix $V^t L V$, because in this case $\lambda_{\min}(V^t L V) = \lambda_2(L) > 0$ (cf. Lemma 7 (iii)) and

$$\gamma(G) := \text{cond}_2(V^t L V) = \frac{\lambda_n}{\lambda_2}.$$

Theorem 8 shows that

$$\sigma_\infty(G) \geq \left\lfloor \frac{n}{\gamma(G)} \right\rfloor$$

and Corollary 12 yields the following bound for balanced separators:

$$|S_3| \geq n \text{h}(\gamma(G))$$

where

$$h(x) := 1 + \frac{9}{16} \frac{(x-1)^2}{x} - \sqrt{\left(1 + \frac{9}{16} \frac{(x-1)^2}{x}\right)^2 - 1}.$$

Other lower bounds for the size of vertex separators can be found in [15] and in [13, Theorem 2.8]. With $\Delta = \Delta(G)$ being the maximal (weighted) degree of G , the latter bound reads

$$|S_3| \geq \frac{4\lambda_2|S_1||S_2|}{\Delta n - \lambda_2|S_1 \cup S_2|}. \quad (21)$$

It is easy to see that (20) is superior to (21) if and only if

$$\lambda_n \leq \Delta + \lambda_2 \left(1 + \frac{m_3}{n} - \frac{\lambda_2}{\lambda_n}\right). \quad (22)$$

For a probabilistic comparison of the obtained bounds, we state another result from [11]. Let $\mathcal{G}_{n,p}$ be the probability space of random graphs of order n with edge probability p .

Theorem 13 *For fixed edge probability p ($0 < p < 1$) and any $\varepsilon > 0$, almost all graphs in $\mathcal{G}_{n,p}$ have their Laplacian eigenvalues $\lambda_2(G)$ and $\lambda_n(G)$ bounded by*

$$pn - f_\varepsilon(n) < \lambda_2 < pn - f_{-\varepsilon}(n)$$

and

$$pn + f_\varepsilon(n) > \lambda_n > pn + f_{-\varepsilon}(n)$$

where $f_\varepsilon(n) = \sqrt{(2 + \varepsilon)p(1 - p)n \log n}$.

Furthermore, we observe that for fixed edge probability p , almost all graphs have $\Delta \geq np$. First we want to show that

$$\left(1 + \frac{m_3}{n} - \frac{\lambda_2}{\lambda_n}\right) \geq \frac{p}{2}$$

for almost all graphs. Note that $1 \geq \lambda_2/\lambda_n$. By a result of Fiedler [4, Theorem 4.1], $\lambda_2 \leq m_3$ and m_3/n can be bounded from below by

$$\lim_{n \rightarrow \infty} \frac{\lambda_2}{n} \geq p - \lim_{n \rightarrow \infty} \frac{f_\varepsilon}{n} = p$$

which proves the claim. We are now ready to show that for fixed edge probability p , (22) is true for almost all graphs. It follows from

$$pn + f_\varepsilon(n) \leq pn + (pn - f_\varepsilon(n)) \frac{p}{2}$$

which is equivalent to

$$f_\varepsilon(n) \left(1 + \frac{p}{2}\right) \leq n \cdot \frac{p^2}{2}.$$

The latter inequality is true for almost all graphs as $f_\varepsilon(n)$ grows slower than n . This proves the following:

Theorem 14 *For fixed edge probability p ($0 < p < 1$), almost all graphs in $\mathcal{G}_{n,p}$ satisfy*

$$\frac{4\lambda_n\lambda_2|S_1||S_2|}{n(\lambda_n - \lambda_2)^2} \geq \frac{4\lambda_2|S_1||S_2|}{\Delta n - \lambda_2|S_1 \cup S_2|}.$$

5 Testing for Subgraph Isomorphism

The problem of subgraph isomorphism can be stated as follows. Given two undirected, unweighted graphs $G = (V, E)$ and $H = (V_H, E_H)$, does G contain a subgraph $G' = (V', E')$ which is isomorphic to H . This problem contains a number of other well known problems such as maximum clique-size, maximum independent set, hamiltonian circuit, etc. In the following, we assume that both graphs G and H are of order n . (Otherwise we add as many isolated vertices as necessary to the smaller graph.) The following lemma is easily proved.

Lemma 15 *Let G and H be unweighted graphs of order n . Let A_G and A_H be the corresponding adjacency matrices. Then G contains a subgraph isomorphic to H if and only if*

$$\max_{X \in \Pi} \text{tr } A_G X A_H X^t = 2|E(H)|.$$

The lemma suggests the following definitions. A graph is a *common subgraph* of two graphs G and H if it is isomorphic to subgraphs of G and H . A graph G' is a *largest common subgraph* of two graphs G and H if it is a common subgraph of G and H and there is no common subgraph with more edges than G' . It is convenient to define the cardinality of the edge set of a common subgraph as the *size* of the common subgraph. Lemma 15 now generalizes to:

Lemma 16 *Let G and H be unweighted graphs of order n . Let A_G and A_H be the corresponding adjacency matrices. Then the size S of a largest common subgraph satisfies*

$$S = \frac{1}{2} \max_{X \in \Pi} \text{tr } A_G X A_H X^t. \quad (23)$$

Note that (23) is symmetric in G and H . If we use the Laplacian L_G instead of A_G , (23) transforms to

$$S = -\frac{1}{2} \min_{X \in \Pi} \text{tr } L_G X A_H X^t. \quad (24)$$

We can now state the main result of this section.

Theorem 17 *Given unweighted graphs G and H of order n , let $L(G)$ and $L(H)$ denote their Laplacian matrices, and let $A(G), A(H)$ be their adjacency matrices, respectively. Then the size S of a largest common subgraph of G and H is bounded by*

$$S \leq \min \left\{ \frac{1}{2} \sum_{i=1}^{n-1} \lambda_{i+1}(L(G)) \lambda_i(-V^t A(H) V), \frac{1}{2} \sum_{i=1}^{n-1} \lambda_{i+1}(L(H)) \lambda_i(-V^t A(G) V) \right\} \quad (25)$$

Proof. The argument is similar to the proof of Theorem 9 and is therefore omitted. \square

The problem of finding the largest, or at least a large common subgraph, has practical applications in distributed computing. Bokhari [1] studies the mapping of finite element grids to an array of processors. If adjacent modules of the grid should also be mapped to directly linked

processors, this leads precisely to the problem of finding the largest common subgraph of the connection structure of the processors and the finite element grid.

Another typical question in graph theory is, given a set E of forbidden edges between vertices labeled from 1 to n , is it possible to label the vertices of a given graph G in such a way that the resulting graph does not contain any edge from E . Let H be the graph of forbidden edges, and let A_G and A_H be the adjacency matrices of G and H , respectively. Then such a labeling for G exists if and only if

$$\min_{X \in \Pi} \operatorname{tr} A_G X A_H X^t = 0. \quad (26)$$

6 Lower bound on the 1-sum problem

The 1-sum $\sigma_1(G)$ of a graph G of order n is defined as

$$\sigma_1(G) := \min \left\{ \sum_{(i,j) \in E} |\phi(i) - \phi(j)| : \phi \text{ bijection } V(G) \rightarrow \{1, \dots, n\} \right\}. \quad (27)$$

Juvan and Mohar [10] formulated the following eigenvalue lower bound depending on the second smallest Laplacian eigenvalue:

$$\sigma_1(G) \geq \lambda_2(L) \frac{n^2 - 1}{6}. \quad (28)$$

We will derive a tighter lower bound based on Theorem 6. Let $B = (b_{ij})$ be an $n \times n$ matrix defined by $b_{ij} = |i - j|$ for every i, j . We recall that $L = L(G)$ denotes the (weighted) Laplacian matrix of a graph G , and V is an $n \times (n - 1)$ projection matrix satisfying (6). We first present some properties of the matrix B .

Lemma 18 *For every n , the above matrix B has the following properties:*

- (i) $\operatorname{tr}(V^t B V) = -\frac{1}{3}(n^2 - 1)$.
- (ii) *The matrix $V^t B V$ is negative definite.*

Proof. (i) Using the properties of V , we have

$$\operatorname{tr} V^t B V = \operatorname{tr} B V V^t = \operatorname{tr} B \left(I - \frac{u u^t}{n} \right) = -\frac{1}{n} u^t B u.$$

It is easily seen that $u^t B u = \sum_{i,j} b_{ij} = \frac{1}{3}(n^3 - n)$. Thus (i) follows.

(ii) Let x be a nonzero vector, and $x \perp u$. We have to show that $x^t B x < 0$. We first note that the vectors $\eta_i := e_i - e_{i+1} = (0, \dots, 0, 1, -1, 0, \dots, 0)^t$ for $i = 1, \dots, n - 1$ form a basis of u^\perp . Thus x can be written as $x = \sum_i a_i \eta_i$ and $\sum_i a_i^2 > 0$. Now note that $\eta_i^t B \eta_j = -2$, if $i = j$, and 0 otherwise. Therefore,

$$x^t B x = \sum_{i,j} a_i a_j \eta_i^t B \eta_j = -2 \sum_i a_i^2 < 0.$$

□

Now we show that Theorem 6 leads to a lower bound on the 1-sum that dominates the Juvan–Mohar bound.

Theorem 19 *Let G be a graph of order n . Then*

$$\sigma_1(G) \geq -\frac{1}{2} \sum_{i=1}^{n-1} \lambda_{i+1}(L) \lambda_i(V^t B V) \geq \frac{n^2 - 1}{6} \lambda_2(L). \quad (29)$$

Moreover, if G is different from the empty and the complete graph, then the second inequality is strict.

Proof. Let $\alpha_i = \lambda_{i+1}(L)$, $i = 1, \dots, n - 1$. By Theorem 6,

$$\sigma_1(G) = -\frac{1}{2} \max\{\text{tr} L X B X^t : X \in \Pi\} \geq -\frac{1}{2} \sum_{i=1}^{n-1} \alpha_i \lambda_i(V^t B V).$$

To demonstrate the second inequality we use the fact that the eigenvalues of $V^t B V$ are negative (Lemma 18(ii)) to conclude

$$-\sum_{i=1}^{n-1} \alpha_i \lambda_i(V^t B V) \geq -\alpha_1 \sum_{i=1}^{n-1} \lambda_i(V^t B V) = \alpha_1 \frac{n^2 - 1}{3}. \quad (30)$$

The last equality follows from Lemma 18(i). Note that $\alpha_1 \neq \alpha_{n-1}$ if G is neither complete nor empty, showing that strict inequality holds in this case. \square

6.1 The 1-sum of Q_n

Let Q_n denote the n -dimensional Cartesian cube. We compare the lower bound of Theorem 19 with the actual value of $\sigma_1(Q_n)$, and with the lower bound (28). The actual value

$$\sigma_1(Q_n) = 2^{n-1}(2^n - 1) \quad (31)$$

was determined by Harper [9]. The Laplacian eigenvalues of Q_n are recalled in Subsection 7.3. The Juvan-Mohar bound states

$$\sigma_1(Q_n) \geq \frac{1}{3}(2^{2n} - 1).$$

The computation of the lower bound of Theorem 19 was done in Matlab, and the results are compared in Table 1. The columns are: the dimension of the cube, Juvan-Mohar bound, bound by Theorem 19, and the exact value by (31).

6.2 The 1-sum in randomly generated graphs

We compare the Juvan-Mohar bound (28) and the bound of Theorem 19 on randomly generated graphs with edge probability 0.5. We have generated 100 graphs for each order $n = 20, 30, \dots, 100$. For each generated graph, we compared the Juvan-Mohar bound (28) and the bound of Theorem 19, respectively. In all cases, the new bound was better than the old one. For each size $n = 20, 30, \dots, 100$, we have computed the average, minimum, and maximum gain of Theorem 19 over

n	Juvan-Mohar	Theorem 19	1-sum
1	1	1	1
2	5	6	6
3	21	24	28
4	85	99	120
5	341	392	496
6	1365	1542	2016
7	5461	6074	8128

Table 1: 1-sum of the cube Q_n

(28). The results are summarized in Table 2. They show the percentage of the improvement, e.g., the number 23.37 in Table 2 means that on 20-vertex examples, the new bound gave 23.37% higher values in average. Let us comment that the high value in the column ‘max’ for small n is caused by the fact that λ_2 is very small when G is not sufficiently connected. (For that reason, only connected graphs were generated.)

n	average	max	min
20	23.37	90.55	9.48
30	13.55	34.99	7.07
40	10.22	35.38	4.61
50	8.07	18.41	3.50
60	6.52	19.82	3.62
70	5.64	16.26	3.07
80	4.81	12.89	2.34
90	4.11	11.08	2.30
100	3.84	8.64	2.05

Table 2: Comparison of bounds on 1-sum for randomly generated graphs

7 Computation and performance of the bounds

In this section we discuss the computability and the performance of the bounds on the bandwidth. We compare the new bounds given in this paper with several previously known results.

7.1 Convexity and persymmetric matrices

Theorem 9 provides a lower bound on the bandwidth. Given a graph G , it is natural to ask what is the best possible lower bound ensured by this theorem. We show that the bound can be computed efficiently for any weighted Laplacian of G . This follows from the fact that, for every k , we can decide in polynomial time whether (9) holds for some $B \in \mathcal{B}_k$. The latter question can be decided by solving the optimization problem

$$\min_{B \in \mathcal{B}_k} f(B) \tag{32}$$

where the function $f(B)$ is defined as

$$f(B) = \sum_{i=1}^{n-1} \alpha_i \lambda_i(V^t B V) \tag{33}$$

where $\alpha_i = \lambda_{i+1}(L)$ are the non-trivial eigenvalues of the Laplacian under an arbitrary (but fixed) weighting of the edges. Using the Fan's theorem and the Rayleigh's principle, it is not difficult to show that $f(B)$ is a convex function. Since the set \mathcal{B}_k is convex as well, problem (32) can be solved in polynomial time by the ellipsoid method (see [7]).

We recall that a matrix $B = (b_{ij})$ is called *persymmetric* if $b_{ij} = b_{n-j+1, n-i+1}$ for every i and j . Using the permutation matrix $T = (t_{ij})$ with $t_{i, n+1-i} = 1$, $i = 1, \dots, n$, it is clear that B is persymmetric if and only if $B = T^t B T$. A consequence of the convexity is that it is enough to consider (32) only on the subclass of persymmetric matrices instead of the whole \mathcal{B}_k . This can be seen as follows: Given B , let B' be defined as $b'_{i,j} = b_{n-j+1, n-i+1}$ for every $i, j = 1, \dots, n$. Clearly, $B \in \mathcal{B}_k$ if and only if $B' \in \mathcal{B}_k$. Moreover, $f(B) = f(B')$ because $V^t B V$ and $V^t B' V$ have the same spectrum. Hence $f(\frac{1}{2}(B + B')) \leq \frac{1}{2}(f(B) + f(B')) = f(B)$ by the convexity. Since $\frac{1}{2}(B + B')$ is persymmetric, the claim follows.

Theorem 9 provides us with a possibility to formulate explicit lower bounds on the bandwidth by specifying a subclass of \mathcal{B}_k . Possible candidates for these subclasses could be either *Toeplitz matrices* ($b_{ij} = c_{|i-j|}$), or *circulant matrices*. The main computational advantage in using circulant matrices consists in the fact that the eigenvalues of a circulant matrix are given by a simple formula (and hence can be computed in an easier way). The disadvantage of course lies in the fact that we have only $n - 2k$ degrees of freedom to choose the circulants.

7.2 The bandwidth of the Petersen graph

We use our results to show that the bandwidth of the Petersen graph is 5. This can be seen as follows. The Laplacian eigenvalues of the Petersen graph are 0, 2, and 5 with multiplicities 1, 5, and 4, respectively. The symmetric Toeplitz matrix having the first row (0 0 0 0 0 4 8 11 14 20) lies in \mathcal{B}_4 and makes (19) negative. This shows a lower bound of 5. On the other hand, it is easy to find a labeling realizing this bound. For comparison, Theorem 8 gives a weaker lower bound 3 on the bandwidth of the Petersen graph.

7.3 The bandwidth of Q_n

Let Q_n denote the n -dimensional Cartesian cube. We compare the lower bound of Theorem 8 with the actual value of $\sigma_\infty(Q_n)$. We show that the lower bound is $\sigma_\infty(Q_n) \geq \frac{2^n}{n} - 1$ while the actual value is $\sigma_\infty(Q_n) \approx 2^n/\sqrt{n}$, which is a relatively narrow gap.

Here are more details. The actual value

$$\sigma_\infty(Q_n) = \sum_{k=0}^{n-1} \binom{k}{\lceil k/2 \rceil} \quad (34)$$

was determined by Harper [9]. Since $\binom{k}{\lceil k/2 \rceil} \approx 2^k/\sqrt{k}$, (34) can be estimated by the double of the largest term. The Laplacian spectrum of Q_n consists of $n+1$ distinct eigenvalues $\mu_i = 2i$, each of multiplicity $\binom{n}{i}$, $i = 0, \dots, n$. (This follows easily from the description of the adjacency spectra of Q_n , see, e.g., [18].) In particular, we have $\lambda_2 = 2$ and $\lambda_{\max} = 2n$. Hence $\sigma_\infty(Q_n) \geq \frac{2^n}{n} - 1$ by Theorem 8.

7.4 The bandwidth of random regular graphs

Though Theorem 8 provides a weaker lower bound on the bandwidth than Theorem 9, it is sufficient to derive the following result of F. de la Vega on the bandwidth of random regular graphs of fixed degree.

Corollary 20 [3] *Almost all d -regular graphs on n vertices have bandwidth at least $b_d n$ where b_d tends to 1 as $d \rightarrow \infty$.*

Proof. It is known [5] that random d -regular graphs have λ_2 bounded away from zero. By Theorem 8 this implies the existence of the constant b_d since $\lambda_n \leq 2d$. Friedman, Kahn, and Szemerédi [5] also proved that for a random d -regular graph G we have $\lambda_2(G) = d - O(\sqrt{d})$ and $\lambda_n(G) = d + O(\sqrt{d})$ with probability tending to 1 as n grows. This shows that $b_d \rightarrow 1$ as $d \rightarrow \infty$.

□

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