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Upper bounds on algebraic connectivity via convex optimization ☆

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Abstract

The second smallest eigenvalue of the Laplacian matrix L of a graph is called its algebraic connectivity. We describe a method for obtaining an upper bound on the algebraic connectivity of a family of graphs $\mathcal{G}$. Our method is to maximize the second smallest eigenvalue over the convex hull of the Laplacians of graphs in $\mathcal{G}$, which is a convex optimization problem. By observing that it suffices to optimize over the subset of matrices invariant under the symmetry group of $\mathcal{G}$, we can solve the optimization problem analytically for families of graphs with large enough symmetry groups. The same method can also be used to obtain upper bounds for other concave functions, and lower bounds for convex functions of L (such as the spectral radius).

1. Introduction

Let $G = (V, E)$ be an undirected graph with n nodes and m edges, and no multiple edges or self-loops. The Laplacian $L(G)$ of G is the (symmetric) matrix

$$L(G)_{ij} = \begin{cases} d_i & i = j, \\ -1 & (i, j) \in E, \quad i \neq j, \\ 0 & (i, j) \notin E, \end{cases}$$

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where d_i is the degree of node i. The Laplacian $L(G)$ satisfies

$$L(G) = L(G)^{\mathrm{T}},\ L(G) \succeq 0,\ L(G)\mathbf{1} = 0,\ L(G)_{ij} \in \{0, -1\} \quad \text{for } i \neq j, \tag{1}$$

where $\succeq$ denotes matrix inequality, and $\mathbf{1}$ is the vector of all ones. In other words, the Laplacian is symmetric positive semidefinite, each row sums to zero, and its off-diagonal elements are either zero or minus one. Conversely, if L is any $n \times n$ matrix that satisfies these conditions, then it is the Laplacian of some graph on n nodes. We will denote the set of all Laplacians on n nodes as $\mathscr{L}$:

$$\mathscr{L} = \{L \in \mathbf{R}^{n\times n} | L = L^{\mathrm{T}}, L \succeq 0, L\mathbf{1} = 0, L_{ij} \in \{0, -1\} \quad \text{for } i \neq j\}.$$

We denote the eigenvalues of a Laplacian $L(G)$ as $\lambda_1 = 0 \leqslant \lambda_2 \leqslant \cdots \leqslant \lambda_n$. The second-smallest eigenvalue of $L(G)$, λ_2, is called the *algebraic connectivity* of G, and is positive if and only if the graph is connected (see, e.g., [6]). The largest eigenvalue λ_n is the *spectral radius*.

Let $\mathscr{G}$ be a set of graphs on n nodes, and let $\mathscr{L}(\mathscr{G}) = \{L(G) \mid G \in \mathscr{G}\}$ be the associated set of Laplacian matrices. We are interested in finding an upper bound on the algebraic connectivity of the graphs in $\mathscr{G}$. In principle, we can compute the maximum algebraic connectivity,

$$\lambda^\star = \max\{\lambda_2(L) | L \in \mathscr{L}(\mathscr{G})\},$$

by evaluating $\lambda_2(L(G))$ for each $G \in \mathscr{G}$. The sets of graphs we are interested in can be extremely large, however, so this is not practical; we seek instead a simple upper bound that depends on some parameters in the description of $\mathscr{G}$.

1.1. Previous work

The Laplacian matrix and its spectrum, particularly the algebraic connectivity and the spectral radius, have been extensively studied. A survey of results and applications can be found in [19] and [21,22] discusses applications of the Laplacian in various fields. The work of Fiedler [6] is one of the earliest addressing the Laplacian matrix, and contains many fundamental results, including upper and lower bounds on the algebraic connectivity. For example, Fiedler shows that

$$\lambda_2(L(G)) \leqslant \frac{nd_{\min}}{n-1} \leqslant \frac{2m}{n-1}, \tag{2}$$

where $d_{\min}$ is the minimum degree of the nodes of G, and that

$$\lambda_2(L(G)) \leqslant v(G), \tag{3}$$

where $v(G)$ is the vertex connectivity, i.e., the minimum number of nodes that need to be deleted to disconnect the graph. (Our method will reproduce all three inequalities.)

Many other upper bounds on $\lambda_2(L)$ have been found in terms of various properties of the graph. In [15] and [14], the author provides tight upper bounds for the algebraic connectivity of a graph with a given number of cut-points. (A cut-point is a vertex whose deletion disconnects the graph). In [7], the authors minimize and maximize $\lambda_2(L)$ for trees of given diameter, and minimize $\lambda_2(L)$ for general graphs of given girth (which is the length of the shortest cycle in the graph). In [8], an upper bound is established in terms of the minimum edge density. The recent work in [16] derives an upper bound for the algebraic connectivity in terms of the domination number of the graph, i.e., the cardinality of the smallest set S such that every element of $V(G)\backslash S$ is adjacent to a vertex of S.

The problem of obtaining lower bounds for the algebraic connectivity and upper bounds for the spectral radius of the Laplacian in terms of various properties of the graph has also been studied; see, for example, [12,17,18,25,20,13].

A closely related problem, which arises in the study of Markov chains and various iterative processes, concerns the matrices $I - D^{-1}L$ and $D^{-1/2}LD^{-1/2}$, where D is the diagonal matrix of node degrees, i.e., $D_{ii} = L_{ii}$. Here the objective is to find upper bounds on the spectral gap of the stochastic matrix $I - D^{-1}L$, which is the same as $\lambda_2(D^{-1/2}LD^{-1/2})$, in terms of various graph properties; see, for example [3,5,13] and references therein.

2. Our method

2.1. The basic bound

Our method for finding a bound on $\lambda^\star$ is simple. We observe that

$$\lambda^\star = \max\{\lambda_2(L) | L \in \mathscr{L}(\mathscr{G})\} \leqslant \bar{\lambda} = \sup\{\lambda_2(L) | L \in \mathbf{Co}\,\mathscr{L}(\mathscr{G})\},$$

where **Co** denotes convex hull. This inequality follows immediately from $\mathbf{Co}\,\mathscr{L}(\mathscr{G}) \supseteq \mathscr{L}(\mathscr{G})$. We will evaluate $\bar{\lambda}$, exploiting the fact that it is the supremum of a concave function over a convex set. Thus, to evaluate $\bar{\lambda}$ requires solving a *convex optimization problem*, i.e., maximizing a concave function over a convex set. Roughly speaking, such problems are easy to solve (in most cases) using numerical methods [2]. Here, however, we will consider cases where the problem can be solved analytically.

To see that λ_2 is a concave function of L on $\mathbf{Co}\,\mathscr{L}$ (and therefore on $\mathbf{Co}\,\mathscr{L}(\mathscr{G})$ for any $\mathscr{G}$), we argue as follows. Each $L \in \mathbf{Co}\,\mathscr{L}$ is positive semidefinite, and has $\lambda_1(L) = 0$, with corresponding eigenvector $\mathbf{1}$. Thus we can express $\lambda_2(L)$ as [11, §4.2]

$$\lambda_2(L) = \inf\{x^{\mathrm{T}}Lx | \|x\|_2 = 1, \mathbf{1}^{\mathrm{T}}x = 0\}.$$

For each $x \in \mathbf{R}^n$ that satisfies $\|x\|_2 = 1$ and $\mathbf{1}^{\mathrm{T}}x = 0$, $x^{\mathrm{T}}Lx$ is a linear (and therefore also concave) function of L. The formula above shows that λ_2 is the infimum of a family of concave functions in L, and is therefore also a concave function of L [2, §3.2.3]. For future use, we note that $\mathbf{Co}\,\mathscr{L}$, the convex hull of the set of all Laplacians on n nodes, has the form

$$\mathbf{Co}\,\mathscr{L} = \{L \in \mathbf{R}^{n\times n} | L = L^{\mathrm{T}}, L \succeq 0, L\mathbf{1} = 0, -1 \leqslant L_{ij} \leqslant 0 \quad \text{for } i \neq j\}, \tag{4}$$

i.e., it is the set of symmetric positive semidefinite matrices, with zero row sums, and off-diagonal elements between minus one and zero.

2.2. Exploiting symmetry

The symmetry group of $\mathscr{G}$ can be exploited to reduce the size of the convex optimization problem that we must solve to evaluate our bound $\bar{\lambda}$. The idea of exploiting symmetry in convex optimization problems has recently found strong interest; see [24,4].

Let $\mathscr{P}$ denote the group of permutation matrices in $\mathbf{R}^{n\times n}$. An element $P \in \mathscr{P}$ acts on a matrix L as PLP^{T}. If L is the Laplacian of a graph G, then PLP^{T} is the Laplacian of the graph $\overline{G}$ obtained by permuting the nodes of G by P. Let $\mathscr{S}$ be the symmetry group of $\mathscr{L}(\mathscr{G})$, i.e.,

$$\mathscr{S} = \{P \in \mathscr{P} | PLP^{\mathrm{T}} \in \mathscr{L}(\mathscr{G}) \text{ for each } L \in \mathscr{L}(\mathscr{G})\}. \tag{5}$$

The group of permutations $\mathscr{S}$ also leaves $\mathbf{Co}\,\mathscr{L}(\mathscr{G})$ invariant. (In what follows, we will only use the fact that $\mathscr{S}$ is *a* group of permutations that leaves $\mathscr{L}(\mathscr{G})$ invariant i.e., it can be a subgroup of the symmetry group.)

Let $\mathscr{I}$ denote the subspace of symmetric $n \times n$ matrices that are invariant under $\mathscr{S}$, i.e.,

$$\mathscr{I} = \{M \in \mathbf{R}^{n\times n} | M = M^{\mathrm{T}},\ PMP^{\mathrm{T}} = M \quad \text{for all } P \in \mathscr{S}\}. \tag{6}$$

We claim that

$$\bar{\lambda} = \sup\{\lambda_2(L) | L \in \mathbf{Co}\,\mathscr{L}(\mathscr{G}) \cap \mathscr{I}\}. \tag{7}$$

In other words, to maximize λ_2 over $\mathbf{Co}\,\mathscr{L}(\mathscr{G})$, we can without loss of generality restrict our search to elements of $\mathbf{Co}\,\mathscr{L}(\mathscr{G})$ that are invariant under $\mathscr{S}$ (see, e.g., [2, Example 4.4]).

To show this, suppose that $L^\star \in \mathbf{Co}\,\mathscr{L}(\mathscr{G})$ satisfies $\lambda_2(L^\star) = \bar{\lambda}$, i.e., $L^\star$ achieves the maximum value of λ_2 over $\mathbf{Co}\,\mathscr{L}(\mathscr{G})$. (Such an $L^\star$ exists because λ_2 is continuous and $\mathbf{Co}\,\mathscr{L}(\mathscr{G})$ is compact.) Now define

$$\overline{L} = \frac{1}{|\mathscr{S}|} \sum_{P \in \mathscr{S}} PL^\star P^{\mathrm{T}}. \tag{8}$$

Clearly $\overline{L} \in \mathbf{Co}\,\mathscr{L}(\mathscr{G})$. Since

$$\lambda_2(PL^\star P^{\mathrm{T}}) = \lambda_2(L^\star) = \bar{\lambda}$$

for any permutation matrix P, and λ_2 is a concave function, Jensen's inequality and (8) tell us that

$$\lambda_2(\overline{L}) \geqslant \lambda_2(L^\star) = \bar{\lambda}. \tag{9}$$

It follows that $\overline{L}$ also maximizes λ_2 over $\mathbf{Co}\,\mathscr{L}(\mathscr{G})$. Our claim (7) is established, since $\overline{L} \in \mathscr{I}$.

3. Examples

In each of the following subsections, we carry out our method of obtaining an upper bound on the algebraic connectivity for a specific set $\mathscr{G}$ of graphs. We start by identifying the symmetry group $\mathscr{S}$ of $\mathscr{G}$. We then identify $\mathscr{I}$, the set of matrices invariant under $\mathscr{S}$, and finally, we evaluate $\bar{\lambda}$ using (7).

3.1. Degree distribution constraints

We start with a simple example where the symmetry group is the set of all permutation matrices. We consider graphs specified by constraints on the degree distribution, i.e.,

$$d_{[1]}, d_{[2]}, \ldots, d_{[n]},$$

which are the degrees of the nodes sorted in decreasing order. (Thus, $d_{[r]}$ denotes the rth largest degree of a node in the graph.)

For any family of graphs $\mathscr{G}$ specified by constraints on the degree distribution, the symmetry group of $\mathscr{L}(\mathscr{G})$ is $\mathscr{P}$, since every permutation leaves the degree distribution, i.e., $d_{[i]}$, unchanged. The subspace $\mathscr{I}$ of symmetric matrices invariant under $\mathscr{P}$ consists of matrices with a constant value along the main diagonal, and a constant value for the off-diagonal elements. Therefore, from (4), we have

$$\mathbf{Co}\,\mathscr{L} \cap \mathscr{I} = \{L | L = n\alpha I - \alpha \mathbf{1}\mathbf{1}^{\mathrm{T}},\ 0 \leqslant \alpha \leqslant 1\}. \tag{10}$$

We now consider a specific constraint on the degree distribution, and find $\bar{\lambda}_2$ for this family of graphs. Let $\mathscr{G}$ be the set of graphs for which the sum of the r largest degrees does not exceed D_r, i.e.,

$$d_{[1]} + d_{[2]} + \cdots + d_{[r]} \leqslant D_r.$$

Clearly we can assume $0 \leqslant D_r \leqslant r(n-1)$. We can express this constraint in terms of L as

$$L_{ii_{[1]}} + L_{ii_{[2]}} + \cdots + L_{ii_{[r]}} \leqslant D_r, \tag{11}$$

where $L_{ii_{[j]}}$ is the jth largest diagonal entry of L. This constraint is convex [2, §3.2.3]. Therefore, $\mathbf{Co}\,\mathscr{L}(\mathscr{G}) \cap \mathscr{I}$ is the subset of matrices in $\mathbf{Co}\,\mathscr{L} \cap \mathscr{I}$ that satisfy (11), i.e.,

$$\mathbf{Co}\,\mathscr{L}(\mathscr{G}) \cap \mathscr{I} = \{L | n\alpha I - \alpha \mathbf{1}\mathbf{1}^{\mathrm{T}},\ 0 \leqslant \alpha \leqslant 1,\ r(n-1)\alpha \leqslant D_r\}. \tag{12}$$

The eigenvalues of the matrix $n\alpha I - \alpha\mathbf{1}\mathbf{1}^{\mathrm{T}}$ are 0, and $n\alpha$ with multiplicity $n-1$, which increase monotonically with α. So to maximize λ_2 over $\mathbf{Co}\,\mathscr{L}(\mathscr{G}) \cap \mathscr{I}$, we set $\alpha = D_r/(n-1)r$. This gives us the bound

$$\bar{\lambda} = \frac{nD_r}{r(n-1)}. \tag{13}$$

A special case of (11) is $r = n$, $D_r = 2m$. Using this in (13) gives us a bound on the algebraic connectivity of graphs with at most m edges,

$$\bar{\lambda} = \frac{2m}{n-1},$$

which recovers the bound in [6].

3.2. *Graphs with small cuts*

We consider graphs in which there exists a cut with no more than m_{c} edges, which breaks the graph into two sets of nodes of sizes n_1 and n_2 (with $n_1 + n_2 = n$). (Note that not every cut separating the graph into sets of size n_1 and n_2 needs to have fewer than m_{c} edges.) We will derive a bound for $\lambda_2(L(G))$ in terms of n_1, n_2, and m_{c}.

We can assume that $0 \leqslant m_{\mathrm{c}} \leqslant n_1 n_2$. Without loss of generality, we label the nodes in the two sets as $\{1, \ldots, n_1\}$ and $\{n_1 + 1, \ldots, n\}$. Thus our set $\mathscr{G}$ consists of graphs for which there are no more than m_{c} edges between the set of nodes $1, \ldots, n_1$ and the set of nodes $n_1 + 1, \ldots, n$. An example is shown in Fig. 1.

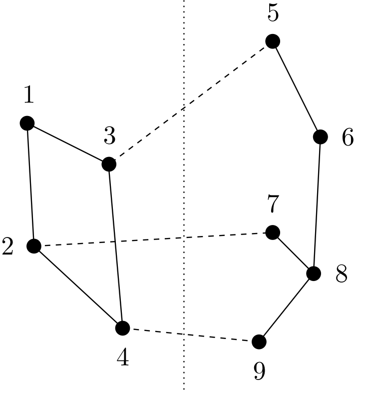

Fig. 1. A graph with a cut (shown as the dotted line) containing three edges (shown as dashed lines). The cut separates nodes $1, \ldots, 4$ from nodes $5, \ldots, 9$. For this graph, we have $m_{\mathrm{c}} = 3$, $n_1 = 4$, and $n_2 = 5$.

In terms of the associated Laplacian matrices, this means that in the 1, 2 $n_1 \times n_2$ block, there are no more than m_c entries that are -1. (The other entries in the block are, of course, zero.) Thus, matrices in $\mathscr{L}(\mathscr{G})$ are the elements of $\mathscr{L}$ that satisfy

$$\sum_{i=1}^{n_1} \sum_{j=n_1+1}^{n} -L_{ij} \leqslant m_c. \tag{14}$$

The symmetry group of $\mathscr{L}(\mathscr{G})$ (for $n_1 \neq n_2$) consists of the matrices

$$P = \begin{bmatrix} P_1 & 0 \\ 0 & P_2 \end{bmatrix}, \tag{15}$$

where P_1 and P_2 are permutation matrices in $\mathbf{R}^{n_1 \times n_1}$ and $\mathbf{R}^{n_2 \times n_2}$ respectively. When $n_1 = n_2$, the symmetry group is larger, consisting of matrices in (15) as well as matrices of the form

$$P = \begin{bmatrix} 0 & P_2 \\ P_1 & 0 \end{bmatrix}.$$

However, this larger symmetry group leads to the same bound as that obtained by setting $n_1 = n_2 = n/2$ in (19), so we do not discuss the case $n_1 = n_2$ separately.

The set $\mathscr{I}$ of matrices that are invariant under $\mathscr{S}$ consists of matrices of the form

$$M = \begin{bmatrix} \alpha I - a\mathbf{1}\mathbf{1}^{\mathrm{T}} & -b\mathbf{1}\mathbf{1}^{\mathrm{T}} \\ -b\mathbf{1}\mathbf{1}^{\mathrm{T}} & \beta I - c\mathbf{1}\mathbf{1}^{\mathrm{T}} \end{bmatrix}, \tag{16}$$

where the vectors of ones are of the appropriate sizes. For a matrix of this form to belong to $\mathscr{L}$, it must have zero row sum, i.e.,

$$\alpha = an_1 + bn_2, \quad \beta = bn_1 + cn_2.$$

Since the off-diagonal entries must lie between 0 and -1, we have $0 \leqslant a, b, c \leqslant 1$. Therefore, from (14), we have

$$\mathbf{Co}\,\mathscr{L}(\mathscr{G}) \cap \mathscr{I} = \{M | 0 \leqslant a, b, c \leqslant 1,\ \alpha = an_1 + bn_2,\ \beta = bn_1 + cn_2,\ bn_1 n_2 \leqslant m_c\}, \tag{17}$$

where M has the structure in (16).

The eigenvalues of a matrix in (17) are shown in the appendix to be

- 0 (with multiplicity one),
- $an_1 + bn_2$ with multiplicity $n_1 - 1$,
- $bn_1 + cn_2$, with mulitplicity $n_2 - 1$,
- $b(n_1 + n_2)$ (with multiplicity one).

Therefore, to maximize the second smallest eigenvalue over $\mathbf{Co}\,\mathscr{L} \cap \mathscr{I}$, we must solve the problem

$$\begin{array}{ll} \text{maximize} & \min\{an_1 + bn_2, bn_1 + cn_2, b(n_1 + n_2)\} \\ \text{subject to} & 0 \leqslant a \leqslant 1, \quad 0 \leqslant c \leqslant 1, \quad 0 \leqslant b \leqslant m_c/n_1 n_2, \end{array} \tag{18}$$

with variables a, b, and c. The objective is non-decreasing in a, b, and c, so the choices $a = 1$, $c = 1$, and $b = m_c/n_1 n_2$ give the optimal value, which is

$$\bar{\lambda} = \frac{m_c(n_1 + n_2)}{n_1 n_2} = \frac{m_c n}{n_1 n_2}. \tag{19}$$

This recovers the bound in [8] and [23],

$$\lambda_2(L) \leqslant \min_{X \subseteq V} \frac{|V||E_X|}{|X||X^c|},$$

where E_X is the number of edges between a subset of nodes X and its complement X^c. The work in [8] addresses the problem of which graphs satisfy this bound with equality.

We also note that Fiedler's bound (2) follows from (19). To see this, choose any node of minimum degree, and consider the cut consisting of its adjacent edges. This cut has size $m_c = d_{\min}$, and disconnects the graph into two sets of nodes, with sizes $n_1 = 1$ and $n_2 = n - 1$. The bound (19) then reduces to Fiedler's bound (2).

3.3. Graphs with non-adjacent subsets

Our next example concerns graphs with no more than m edges, with q non-adjacent, disjoint subsets $S_1, \ldots, S_q$, each containing p nodes. (S_i and S_j are non-adjacent if there are no edges between them.) We denote the remaining $t = n - pq$ nodes as T:

$$T = \{1, \ldots, n\} \backslash (S_1 \cup \cdots \cup S_q).$$

We will derive a bound on $\lambda_2(L(G))$ in terms of m, p, q and t.

Without loss of generality, we can assume that

$$S_1 = \{1, \ldots, p\},\ S_2 = \{p+1, \ldots, 2p\}, \ldots, S_q = \{(q-1)p+1, \ldots, pq\},$$
$$T = \{pq+1, \ldots, n\}.$$

We let $\mathscr{G}$ consist of graphs with this form, with no more than m edges. An example is shown in Fig. 2.

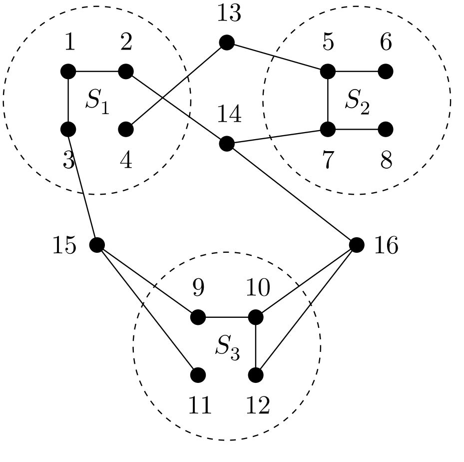

Fig. 2. A graph with $n = 16$ nodes, $m = 17$ edges, and $q = 3$ non-adjacent subsets, S_1, S_2, and S_3, each containing $p = 4$ nodes. The set T consists of the remaining nodes: 13, 14, 15 and 16.

For this $\mathscr{G}$, matrices in $\mathscr{L}(\mathscr{G})$ have the block arrow form

$$L = \begin{bmatrix} L_1 & & & R_1 \\ & \ddots & & \vdots \\ & & L_q & R_q \\ R_1^T & \cdots & R_q^T & L_{q+1} \end{bmatrix}, \tag{20}$$

where $L_i \in \mathbf{R}^{p\times p}$, $i = 1, \dots, q$, $L_{q+1} \in \mathbf{R}^{t\times t}$, and $R_i \in \mathbf{R}^{p\times t}$, and

$$\sum_{i\neq j} -L_{ij} = \sum_{i=1}^{n} L_{ii} \leqslant 2m.$$

(Blocks not shown are zero.)

The set $\mathscr{L}(\mathscr{G})$ is invariant under a permutation of nodes within each subset $S_1, \dots, S_q$ and T, as well as permutations of the q subsets $S_1, \dots, S_q$ amongst themselves. That is, the symmetry group of $\mathscr{L}(\mathscr{G})$ consists of the matrices

$$P = \begin{bmatrix} \tilde{P} & \\ & P_t \end{bmatrix},$$

where P_t is a permutation matrix in $\mathbf{R}^{t\times t}$, and

$$\tilde{P} = (P_q \otimes I_p) \begin{bmatrix} P_p^1 & & \\ & \ddots & \\ & & P_p^k \end{bmatrix}, \tag{21}$$

where P_q and P_p^i are permutation matrices in $\mathbf{R}^{q\times q}$ and $\mathbf{R}^{p\times p}$ respectively, and I_p is the identity matrix in $\mathbf{R}^{p\times p}$. (The symbol $\otimes$ denotes Kronecker product.)

A matrix that is invariant under any permutation in $\mathscr{S}$ is of the form

$$M = \begin{bmatrix} \tilde{\alpha} I - \tilde{a}\mathbf{1}\mathbf{1}^T & -\tilde{b}\mathbf{1}\mathbf{1}^T \\ -\tilde{b}\mathbf{1}\mathbf{1}^T & \tilde{\beta} I - \tilde{c}\mathbf{1}\mathbf{1}^T \end{bmatrix}, \tag{22}$$

where the vectors of ones are of the appropriate sizes.

From (20) and (22), we see that matrices in $\mathbf{Co}\,\mathscr{L}(\mathscr{G}) \cap \mathscr{I}$ are of the form

$$M = \begin{bmatrix} \alpha I - a\mathbf{1}\mathbf{1}^T & & & -b\mathbf{1}\mathbf{1}^T \\ & \ddots & & \vdots \\ & & \alpha I - a\mathbf{1}\mathbf{1}^T & -b\mathbf{1}\mathbf{1}^T \\ -b\mathbf{1}\mathbf{1}^T & \cdots & -b\mathbf{1}\mathbf{1}^T & \beta I - c\mathbf{1}\mathbf{1}^T \end{bmatrix}, \tag{23}$$

where

$$\alpha = ap + bt, \quad \beta = pqb + ct, \quad 0 \leqslant a, b, c \leqslant 1,$$
$$qp(p-1)a + t(t-1)c + 2pqtb \leqslant 2m.$$

The eigenvalues of M are shown in the appendix to be

- 0, with multiplicity 1,
- $ap + bt$, with multiplicity $q(p-1)$,
- $pqb + tc$, with multiplicity $t-1$,
- bt, with multiplicity $q-1$,
- $b(t+qp)$ with multiplicity 1.

Since a and c are non-negative, the second smallest eigenvalue of M is

$$\lambda_2 = \min\{tb, pqb + tc\}.$$

To find the bound $\bar{\lambda}$, we must solve the problem

$$\begin{array}{ll} \text{maximize} & \min\{tb, pqb + tc\} \\ \text{subject to} & 0 \leqslant a, b, c \leqslant 1, \quad qp(p-1)a + t(t-1)c + 2pqtb \leqslant 2m, \end{array} \tag{24}$$

with variables a, b, and c. This is small linear program that we can solve analytically. We start by noting that the objective does not depend on a, and is non-decreasing in b and c. The second inequality is increasing in a, b, and c, so it follows that we should take $a = 0$. To find the optimal values for the two remaining variables b and c, we consider two cases: $pq \geqslant t$, and $pq < t$.

Suppose that $pq \geqslant t$. Then the objective in (24) is bt, so the problem reduces to maximizing b. The optimal value of c is zero, which allows b to be as large as possible, i.e., $b = \min\{m/pqt, 1\}$. This yields the optimal value

$$\bar{\lambda} = \min\{t, m/(pq)\}.$$

Now consider the case when $pq < t$. In this case the two terms in the objective are equal at the optimal point, i.e., $tb = pqb + tc$. Using this in the constraint

$$t(t-1)c + 2pqtb \leqslant 2m,$$

we get

$$b = \min\left\{1, \frac{2m}{(t-1)(t-pq) + 2pqt}\right\}.$$

This gives us

$$\bar{\lambda} = \min\left\{t, \frac{2mt}{(t-1)(t-pq) + 2pqt}\right\}.$$

In summary, we have the following:

$$\bar{\lambda} = \min\left\{t, \frac{2mt}{(t-1)(t-pq)_+ + 2pqt}\right\}, \tag{25}$$

where $(t-pq)_+$ denotes the positive part of $t - pq$, i.e., $\max\{t - pq, 0\}$. This is our final bound for graphs with q non-adjacent subsets, each with p nodes, and no more than m edges.

We can connect our bound to the simple one (3) based on vertex connectivity. The vertex connectivity of any graph in $\mathcal{G}$ is less than or equal to t, since deleting the nodes in T will surely disconnect the graph. Thus the simple bound gives us $\lambda_2(L(G)) \leqslant v(G) \leqslant t$. If in our bound we ignore the constraint on the total number of edges (or just set the number of edges to its largest possible value, $m = n(n-1)/2$), we also obtain

$$\lambda_2(L(G)) \leqslant \bar{\lambda} = t.$$

3.4. Graphs with ring structure

We consider graphs with no more than m edges, with the following block ring structure. The nodes can be divided into $q > 1$ disjoint sets of nodes, $S_1, \ldots, S_q$, each with p nodes ($n = pq$), such that there are edges between sets S_i and S_j only if $|i - j| \leqslant 1$ or $|i - j| = q - 1$. In other words, S_1 can be adjacent only to S_q and S_2, S_2 can be adjacent only to S_1 and S_3, and so on; S_q can be adjacent only to S_{q-1} and S_1. We will derive a bound on $\lambda_2(L(G))$ in terms of m, p and q.

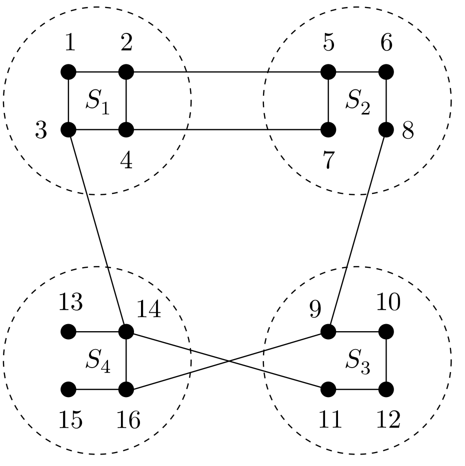

Fig. 3. A graph with $n = 16$ nodes, $m = 19$ edges, and a ring structure with $q = 4$ subsets, $S_1, \ldots, S_4$, each containing $p = 4$ nodes.

Without loss of generality, we can assume that

$$S_1 = \{1, \ldots, p\}, \ldots, S_q = \{(q-1)p+1, \ldots, n\}.$$

Our set $\mathscr{G}$ will be graphs with this structure, with no more than m edges in total. An example is shown in Fig. 3.

Note that if $q < 4$, then this requirement does not impose any structure on the graph, since all of the q subsets are adjacent to each other. Therefore, we will assume for the remainder of this section that $q \geqslant 4$.

For this $\mathscr{G}$, $\mathscr{L}(\mathscr{G})$ is the subset of matrices in (1) that have the form

$$L = \begin{bmatrix} R_{11} & R_{12} & & R_{1q} \\ R_{12}^{\mathrm{T}} & R_{22} & R_{23} & \\ & & \ddots & \\ R_{1q}^{\mathrm{T}} & & R_{qq-1} & R_{qq} \end{bmatrix}, \tag{26}$$

where $R_{ij} \in \mathbf{R}^{p\times p}$, and

$$\sum_{i=1}^{n} L_{ii} \leqslant 2m.$$

(The sparsity structure of L could be called block tridiagonal circulant.)

The set $\mathscr{L}(\mathscr{G})$ is invariant under a permutation of nodes within each of the sets $S_1, \ldots, S_q$, as well as to cyclic rotations of the sets, and reversal of the ordering of the subsets. That is, the symmetry group of $\mathscr{L}(\mathscr{G})$ consists of the permutation matrices

$$P = (\tilde{P} \otimes I_p) \begin{bmatrix} P^1 & & \\ & \ddots & \\ & & P^q \end{bmatrix},$$

where $P^i \in \mathbf{R}^{p\times p}$ are permutation matrices, and $\tilde{P} \in \mathbf{R}^{q\times q}$ is a cyclic permutation or reversal. That is, P is a block cyclic permutation matrix, with every block a permutation matrix in $R^{p\times p}$.

The set of symmetric matrices invariant under S has elements of the form $\alpha I_n - C \otimes \mathbf{1}\mathbf{1}^\mathrm{T}$, where $C \in \mathbf{R}^{q\times q}$ is a symmetric circulant matrix. Therefore, the set of matrices in $\mathbf{Co}\,\mathscr{L}(\mathscr{G}) \cap \mathscr{I}$ has the form

$$M = \alpha I_n - C \otimes \mathbf{1}\mathbf{1}^\mathrm{T}, \tag{27}$$

where C is the circulant matrix

$$C = \begin{bmatrix} a & b & & b \\ b & a & b & \\ & & \ddots & \\ b & & b & a \end{bmatrix}, \tag{28}$$

and

$$\alpha = p(a + 2b); \quad n(p-1)a + 2npb \leqslant 2m.$$

The eigenvalues of C are (see, for example, [10])

$$\mu_j = a + 2b\cos(2\pi j/q), \quad j = 1, \ldots, q.$$

So the eigenvalues of $C \otimes \mathbf{1}\mathbf{1}^\mathrm{T}/n$ are 0 repeated $n-q$ times, and $p\mu_j$, $j = 1, \ldots, q$. Therefore, the eigenvalues of M are

- $ap + 2bp$, with multiplicity $n - q$, and
- $2bp(1 - \cos(2\pi j/q))$, with multiplicity 1, for $j = 1, \ldots, q$.

For $j = q$, $1 - \cos(2\pi j/q) = 0$. The second smallest value of $2pb(1 - \cos(2\pi j/q))$ is obtained for $j = 1$ (or $j = q - 1$). Therefore,

$$\lambda_2 = \min(ap + 2bp, 2bp(1 - \cos(2\pi/q))).$$

For $q \geqslant 4$, $\cos(2\pi/q) \geqslant 0$, and therefore $\lambda_2 = 2bp(1 - \cos(2\pi/q))$, which does not depend on a, and is increasing in b. Therefore, to maximize λ_2 over $\mathbf{Co}\,\mathscr{L}(\mathscr{G}) \cap \mathscr{I}$, we set $a = 0$, and $b = m/np$. This gives us the following upper bound on the algebraic connectivity of graphs with n nodes, no more than m edges, and a block ring structure with $q \geqslant 4$ blocks:

$$\bar{\lambda} = \frac{2m}{n}(1 - \cos(2\pi/q)). \tag{29}$$

When $1 < q < 4$, the same method still works; in this case, we obtain an upper bound on the algebraic connectivity over the set of all graphs with no more than m edges. The bound we obtain here is, once again,

$$\bar{\lambda} = \frac{2m}{n-1}.$$

4. Bounds for other functions

Our method relies only on the fact that $\lambda_2(L)$ is a concave function of L on $\mathbf{Co}\,\mathscr{L}$, which is invariant under any permutation of the nodes. The same method can also be used to obtain an upper bound on any other concave function, or a lower bound on any convex function, which is invariant under node permutation. As above, we can restrict the optimization to the subspace of symmetric matrices invariant under the symmetry group. As examples, the same method can be used to find the following bounds.

- *Spectral radius.* The largest eigenvalue $\lambda_n(L)$ is convex function of L, so by minimizing it over $L \in \mathbf{Co}\,\mathscr{L}(\mathscr{G})$ (which is a convex optimization problem), we obtain a lower bound on $\lambda_n(L)$ over $\mathscr{G}$.
- *Sum of k largest or k smallest eigenvalues.* The sum of the k largest eigenvalues of L,

$$f(L) = \sum_{i=0}^{k-1} \lambda_{n-i}(L)$$

is a convex function of L. Similarly, the sum of the smallest k eigenvalues,

$$g(L) = \sum_{i=2}^{k} \lambda_i(L),$$

is a concave function of L. Therefore, our method can be used to find a lower bound on $f(L)$ and an upper bound on $g(L)$ over a family of graphs $\mathscr{G}$. (For $k = 1$, these functions reduce to the spectral radius and the algebraic connectivity respectively.)
- *Geometric mean of eigenvalues.* The function

$$\left(\prod_{i=2}^{n} \lambda_i\right)^{1/(n-1)}$$

is concave, so we can find an upper bound on it. The same upper bound can also be found by maximizing the concave function

$$\log\det(L + \mathbf{1}\mathbf{1}^{\mathrm{T}}/n) = \sum_{i=2}^{n} \log \lambda_i(L).$$

The product of the largest $n - 1$ eigenvalues of the Laplacian is related to the number of spanning trees in G by the matrix-tree theorem (see, for example, [21]): the number of spanning trees in G, $\kappa(G)$, is given by

$$\kappa(G) = \frac{1}{n} \prod_{i=2}^{n} \lambda_i(L(G)).$$

Thus we can find an upper bound on the number of spanning trees in graphs belonging to some family of graphs $\mathscr{G}$.
- *Total effective resistance.* The total effective resistance of a graph is proportional to

$$\sum_{i=2}^{n} \lambda_i^{-1} = \mathbf{Tr}(L + \mathbf{1}\mathbf{1}^{\mathrm{T}}/n)^{-1} - 1$$

(see [9]). This is a convex function of L, so we can find a lower bound on the total resistance, over a family of graphs, using the method outlined above.
- *Mean-square-variance in distributed averaging.* When a graph is used as a distributed averaging network, with random noises acting on each edge, the total variance of the error is proportional to

$$\sum_{i=2}^{n} \lambda_i^{-2} = \mathbf{Tr}(L + \mathbf{1}\mathbf{1}^{\mathrm{T}}/n)^{-2} - 1$$

(see [26]). This is a convex function of L, so our method can be used to find a lower bound on it.

Each of these functions of L is a *spectral function*, i.e., a symmetric function of the eigenvalues of a symmetric matrix. A spectral function $g(\lambda(L))$ is closed and convex if and only if g is closed and convex; this can be used to show convexity of the functions above. For more on spectral functions, see [1].

Appendix

We want to find the eigenvalues of the matrix

$$L = \begin{bmatrix} \alpha I - a\mathbf{1}\mathbf{1}^{\mathrm{T}} & -b\mathbf{1}\mathbf{1}^{\mathrm{T}} \\ -b\mathbf{1}\mathbf{1}^{\mathrm{T}} & \beta I - c\mathbf{1}\mathbf{1}^{\mathrm{T}} \end{bmatrix}, \tag{30}$$

where α and β satisfy

$$\alpha = an_1 + bn_2, \quad \beta = bn_1 + cn_2. \tag{31}$$

We can diagonalize $\alpha I - a\mathbf{1}\mathbf{1}^{\mathrm{T}}$ as

$$\alpha I - a\mathbf{1}\mathbf{1}^{\mathrm{T}} = \begin{bmatrix} \frac{1}{\sqrt{n_1}}\mathbf{1} & U \end{bmatrix}^{\mathrm{T}} D_1 \begin{bmatrix} \frac{1}{\sqrt{n_1}}\mathbf{1} & U \end{bmatrix}, \tag{32}$$

where $D_1 \in \mathbf{R}^{n_1 \times n_1}$ is the diagonal matrix with entries $\alpha - an_1, \alpha, \ldots, \alpha$, and $U \in \mathbf{R}^{n_1 \times n_1 - 1}$ is an orthonormal basis for $\mathbf{1}^{\perp}$. We can similarly diagonalize $\beta I - c\mathbf{1}\mathbf{1}^{\mathrm{T}}$ as

$$\beta I - c\mathbf{1}\mathbf{1}^{\mathrm{T}} = \begin{bmatrix} \frac{1}{\sqrt{n_2}}\mathbf{1} & V \end{bmatrix}^{\mathrm{T}} D_2 \begin{bmatrix} \frac{1}{\sqrt{n_2}}\mathbf{1} & V \end{bmatrix}, \tag{33}$$

where D_2 has entries $\beta - cn_2, \beta, \ldots, \beta$, and $V \in \mathbf{R}^{n_2 \times n_2 - 1}$ is an orthonormal basis for $\mathbf{1}^{\perp}$.

We have

$$\begin{bmatrix} \frac{1}{\sqrt{n_1}}\mathbf{1} \;\; U & 0 \\ 0 & \frac{1}{\sqrt{n_2}}\mathbf{1} \;\; V \end{bmatrix}^{\mathrm{T}} \begin{bmatrix} \alpha I - a\mathbf{1}\mathbf{1}^{\mathrm{T}} & b\mathbf{1}\mathbf{1}^{\mathrm{T}} \\ b\mathbf{1}\mathbf{1}^{\mathrm{T}} & \beta I - c\mathbf{1}\mathbf{1}^{\mathrm{T}} \end{bmatrix} \times \begin{bmatrix} \frac{1}{\sqrt{n_1}}\mathbf{1} \;\; U & 0 \\ 0 & \frac{1}{\sqrt{n_2}}\mathbf{1} \;\; V \end{bmatrix} = \begin{bmatrix} D_1 & S^{\mathrm{T}} \\ S & D_2 \end{bmatrix}, \tag{34}$$

where $S \in \mathbf{R}^{n_2 \times n_1}$ has $S_{11} = -b\sqrt{n_1 n_2}$, and all other entries zero.

The right-hand side matrix can be permuted to

$$\begin{bmatrix} \alpha - an_1 & -b\sqrt{n_1 n_2} & & \\ -b\sqrt{n_1 n_2} & \beta - cn_2 & & \\ & & \alpha I_{n_1 - 1} & \\ & & & \beta I_{n_2 - 1} \end{bmatrix} = \begin{bmatrix} bn_2 & -b\sqrt{n_1 n_2} & & \\ -b\sqrt{n_1 n_2} & bn_1 & & \\ & & \alpha I_{n_1 - 1} & \\ & & & \beta I_{n_2 - 1} \end{bmatrix}, \tag{35}$$

which has eigenvalues α repeated $n_1 - 1$ times, β repeated $n_2 - 1$ times, 0, and $b(n_1 + n_2)$. Since this block-diagonal matrix is obtained from L by a series of similarity transformations, these are also the eigenvalues of L.

Next we find the eigenvalues of

$$L^\star = \begin{bmatrix} \alpha I - a\mathbf{1}\mathbf{1}^T & & & -b\mathbf{1}\mathbf{1}^T \\ & \ddots & & \vdots \\ & & \alpha I - a\mathbf{1}\mathbf{1}^T & -b\mathbf{1}\mathbf{1}^T \\ -b\mathbf{1}\mathbf{1}^T & \cdots & -b\mathbf{1}\mathbf{1}^T & \beta I - c\mathbf{1}\mathbf{1}^T \end{bmatrix}. \tag{36}$$

By a similarity transform like the one above, this matrix can be transformed to the matrix

$$\begin{bmatrix} D_1 & & & S^T \\ & \ddots & & \vdots \\ & & D_1 & S^T \\ S & \cdots & S & D_2 \end{bmatrix}, \tag{37}$$

where D_1 is diagonal with entries $\alpha - an_1, \alpha, \ldots, \alpha$, D_2 is diagonal with entries $\beta - cn_2, \beta, \ldots, \beta$, and $S \in \mathbf{R}^{n_2 \times n_1}$ has $S_{11} = -b\sqrt{n_1 n_2}$, and all other entries zero.

This matrix can be permuted to a block diagonal matrix

$$\begin{bmatrix} \alpha - an_1 & & & -b\sqrt{n_1n_2} & & \\ & \ddots & & \vdots & & \\ & & \alpha - an_1 & -b\sqrt{n_1n_2} & & \\ -b\sqrt{n_1n_2} & \ldots & -b\sqrt{n_1n_2} & \beta - cn_2 & & \\ & & & & \alpha I_{k(n_1-1)} & \\ & & & & & \beta I_{n_2-1} \end{bmatrix}$$

$$= \begin{bmatrix} bn_2 & & & -b\sqrt{n_1n_2} & & \\ & \ddots & & \vdots & & \\ & & bn_2 & -b\sqrt{n_1n_2} & & \\ -b\sqrt{n_1n_2} & \ldots & -b\sqrt{n_1n_2} & kbn_1 & & \\ & & & & \alpha I_{k(n_1-1)} & \\ & & & & & \beta I_{n_2-1} \end{bmatrix}.$$

The eigenvalues of the top left block can be computed to be 0, bn_2 repeated $k-1$ times, and $b(n_2 + kn_1)$. So the eigenvalues of $L^\star$ (which are the same as those of the above block diagonal matrix) are 0, bn_2 repeated $k-1$ times, $b(n_2+kn_1)$, α repeated $k(n_1-1)$ times, and β repeated $n_2 - 1$ times.

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