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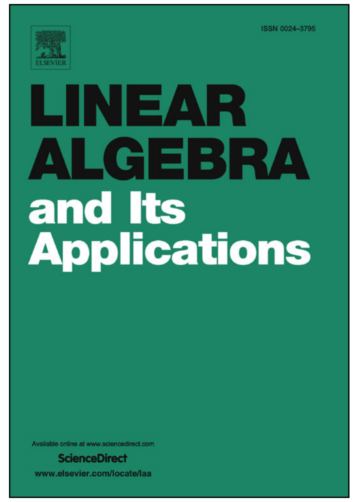

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New Bounds for the Signless Laplacian Spread

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Abstract

Let G be an undirected simple graph. The signless Laplacian spread of G is defined as the maximum distance of pairs of its signless Laplacian eigenvalues. This paper establishes some new bounds, both lower and upper, for the signless Laplacian spread. Several of these bounds depend on invariant parameters of the graph. We also use a minmax principle to find several lower bounds for this spectral invariant.

Keywords:
Matrix spread, signless Laplacian spread, signless Laplacian matrix
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1. Introduction

In this paper we study an spectral invariant called signless Laplacian spread, defined as the difference between the maximum and minimum signless Laplacian eigenvalues. We deal with an undirected simple graph G with vertex set $\mathcal{V}(G)$ of cardinality n and edge set $\mathcal{E}(G)$ of cardinality m; we call this an (n,m)-graph. An edge $e \in \mathcal{E}(G)$ with end vertices u and v is denoted by uv, and we say that u and v are neighbors. A vertex v is incident to an edge e if $v \in e$. $N_G(v)$ is the set of neighbors of the vertex v, and its cardinality is the degree of v, denoted by $d(v)$. Sometimes, after a labeling of the vertices of G, a vertex v_i is simply written i and an edge v_iv_j is written ij, and we write d_i for $d(v_i)$. The minimum and maximum vertex degree of G are denoted by $\delta(G)$ (or simply δ) and $\Delta(G)$ (or simply Δ), respectively. As usual, K_n, C_n and P_n denote, respectively the *complete* graph, the *cycle* and the *path* with n vertices. The *complete bipartite* graph with the part sizes p and q is denoted by $K_{p,q}$. We denote by $G \cup H$ the vertex disjoint union of graphs G and H. We only consider graphs without isolated vertices. Let $d_1, d_2, \ldots, d_n$ be the vertex degrees of G. Denote by $A_G = (a_{ij})$ the adjacency matrix of G. The spectrum of A_G is called the *spectrum* of G and its elements are called the *eigenvalues of* G. The vertex degree matrix D_G is the $n \times n$ diagonal matrix of the vertex degrees d_i of G. The *signless Laplacian matrix* of G (see e.g. [9]) is defined by

$$Q_G = D_G + A_G. \tag{1}$$

So, if $Q_G = (q_{ij})$, then $q_{ij} = 1$ when $ij \in \mathcal{E}(G)$, $q_{ii} = d_i$, and the remaining entries are zero. The signless Laplacian matrix is nonnegative and symmetric. The signless Laplacian spectrum of G is the spectrum of Q_G. Similarly, the matrix

$$L_G = D_G - A_G$$

is the *Laplacian matrix* of G ([9, 16, 17]). For all these matrices we may omit the subscript G if no misunderstanding should arise. Moreover, the matrices Q_G and L_G are positive semidefinite.

For a real symmetric matrix W_G, associated to a graph G, its spectrum (the multiset of the eigenvalues of W_G) is denoted by σ_{W_G}, and we let $\eta_i(W_G)$ denote the i-th largest eigenvalue of W_G. The i-th largest eigenvalue of A_G (L_G, Q_G, respectively) is denoted by $\lambda_i(G)$ ($\mu_i(G)$, $q_i(G)$, respectively). Sometimes they are simply denoted by λ_i (μ_i, q_i, respectively).

Note: We treat vectors in $\mathbf{R}^n$ as column vectors, but identify these with the corresponding n-tuples.

1.1. The spread of symmetric matrices

This subsection collects some general results that are known for the spread of a symmetric matrix.

Let ω_i be the i-th largest eigenvalue of a symmetric matrix W. The *spread* of W is defined by

$$s(W) = \omega_1 - \omega_n.$$

There are several papers devoted to this parameter, see for instance [22, 23, 29, 31]. For a square matrix $W = (w_{ij})$, let $\|W\|_F = (\sum_{ij} |w_{ij}|^2)^{1/2}$ and $\operatorname{tr} W$ be its Frobenius matrix norm and trace, respectively. In 1956, Mirsky proved the following inequality.

Theorem 1. ([29]) *Let W be an $n \times n$ matrix. Then*

$$s(W) \leq \left(2 \|W\|_F^2 - \frac{2}{n} (\operatorname{tr} W)^2\right)^{1/2} \tag{2}$$

with equality if and only if W is normal and the eigenvalues $\omega_1, \omega_2, \ldots, \omega_n$ of W satisfy the following condition

$$\omega_2 = \omega_3 = \cdots = \omega_{n-1} = \frac{\omega_1 + \omega_n}{2}.$$

Concerning lower bounds, among the results obtained for the spread of a symmetric matrix $W = (w_{ij})$, we mention the following obtained in [3].

Theorem 2. ([3]) *Let $W = (w_{ij})$ be an $n \times n$ Hermitian matrix. Then*

$$s(W) \geq \max_{i,j} \left((w_{ii} - w_{jj})^2 + 2 \sum_{s \neq j} |w_{js}|^2 + 2 \sum_{s \neq i} |w_{is}|^2 \right)^{1/2}. \tag{3}$$

Some other lower bounds for the spread of Hermitian matrices are found in [22], and in some cases these improve the lower bound in (3).

Theorem 3. ([22]) *For any Hermitian matrix* $W = (w_{ij})$

$$s(W)^2 \geq \max_{i \neq j} \left\{ (w_{ii} - w_{jj})^2 + 2\sum_{k \neq i} |w_{ik}|^2 + 2\sum_{k \neq j} |w_{jk}|^2 + 4e_{ij} \right\},$$

where $e_{ij} = 2f_{ij}$ *if* $w_{ii} = w_{jj}$ *and otherwise*

$$e_{ij} = \min \left\{ (w_{ii} - w_{jj})^2 + 2 \left| (w_{ii} - w_{jj})^2 - f_{ij} \right|, \frac{f_{ij}^2}{(w_{ii} - w_{jj})^2} \right\}$$

with

$$f_{ij} = \left| \sum_{k \neq i} |w_{ik}|^2 - \sum_{k \neq j} |w_{jk}|^2 \right|.$$

1.2. Spreads associated with graphs

Let G be an (n, m)-graph. We now consider different notions of spread based on matrices associated with G.

As before A_G is the adjacency matrix of G and we consider

$$s(G) = s(A_G)$$

which is called the *spread* of G ([15]). Let $\mu(G) = (\mu_1, \mu_2, \ldots, \mu_n)$ be the vector whose components are the Laplacian eigenvalues of G (ordered decreasingly, as usual). The *Laplacian spread*, denoted by $s_L(G)$, is defined ([41]) by

$$s_L(G) = \mu_1 - \mu_{n-1}.$$

Note that $\mu_n = 0$. Let $q(G) = (q_1, q_2, \ldots, q_n)$ be the vector whose components are the signless Laplacian eigenvalues ordered decreasingly. The *signless Laplacian spread*, denoted by $s_Q(G)$, is defined ([26], [32]) as

$$s_Q(G) = q_1 - q_n.$$

Remark 4. Some basic properties of these notions are as follows:

(i) Let G be a graph of order n with largest vertex degree Δ. From Theorem 2 one can easily see that $s(G) \geq 2\sqrt{\Delta}$. Moreover, if $G = K_{1,n-1}$, equality holds.

(ii) If G is a regular graph, then $s_Q(G) = s(G)$, ([26]).

(iii) From the relation $Q_G = 2A_G + L_G$ it follows that $q_1 \geq 2\lambda_1$ as L_G is positive semidefinite (and it is known that equality holds if and only if G is a regular graph), (see e.g [8, 12]). Moreover, as λ_1 is the spectral radius of A_G, $2\lambda_1 \geq \lambda_1 - \lambda_n = s(G)$ with equality if and only if G is a bipartite graph. Therefore

$$s(G) \leq q_1$$

with equality if and only if G is a regular, bipartite graph.

(iv) We recall the Weyl's inequalities for a particular case in what follows. Consider two $n \times n$ Hermitian matrices W and U with eigenvalues (ordered nonincreasingly) $\omega_1, \omega_2, \ldots, \omega_n$ and $x_1, x_2, \ldots, x_n$, respectively, and the Hermitian matrix $T = W + U$ with eigenvalues $\tau_1, \tau_2, \ldots, \tau_n$ (ordered nonincreasingly). Then the following inequalities hold

$$\omega_n + x_i \leq \tau_i \leq \omega_1 + x_i \quad (i \leq n).$$

Thus $\omega_n + x_1 \leq \tau_1 \leq \omega_1 + x_1$ and $\omega_n + x_n \leq \tau_n \leq \omega_1 + x_n$. Therefore

$$x_1 - x_n + \omega_n - \omega_1 \leq \tau_1 - \tau_n \leq \omega_1 - \omega_n + x_1 - x_n$$

which gives the following inequalities for the spread of these matrices

$$|s(U) - s(W)| \leq s(T) \leq s(W) + s(U).$$

(v) Let G be a graph with minimum and maximum vertex degree δ and Δ, respectively. By the previous item, as $Q_G = D_G + A_G$, $|\Delta - \delta - s(G)| \leq s_Q(G) \leq s(G) + \Delta - \delta$. By all the previous items we conclude that

$$|\ s_Q(G) - s(G)| \leq \Delta - \delta.$$

The next inequality establishes a relation between the largest Laplacian eigenvalue and the largest signless Laplacian eigenvalue.

Lemma 5. ([40]) *Let G be a graph. Then*

$$\mu_1(G) \leq q_1(G).$$

Moreover if G is connected, then the equality holds if and only if G is a bipartite graph.

The second smallest Laplacian eigenvalue of a graph G is known as the algebraic connectivity ([13]) of G and denoted by $a(G)$. If G is a non-complete connected graph, then $a(G) \leq \kappa_0(G)$, where $\kappa_0(G)$ is the vertex connectivity of G (that is, the minimum number of vertices whose removal yields a disconnected graph). Since $\kappa_0(G) \leq \delta(G)$, it follows that $a(G) \leq \delta$. The graphs for which the algebraic connectivity attains the vertex connectivity are characterized in [25]. One also has ([2, 39])

$$s_L(G) \geq \Delta(G) + 1 - \delta(G). \tag{4}$$

For a survey on algebraic connectivity, see [1]. Moreover, it is worth to conclude that the result in (4) together with the result in Remark 4 (v) imply that

$$s_Q(G) \leq s(G) + s_L(G) - 1.$$

Remark 6. If G is a connected (n,m)-graph such that $m \leq n-1$, then G does not have cycles and thus, it is bipartite. Therefore $s_Q(G) = q_1 = \mu_1$. As in the literature there are many known lower and upper bounds for this eigenvalue,see for instance, [28, 35], from now on we only treat the case $m \geq n$.

Some other results on $s_Q(G)$ can be found, for instance, in [26, 32, 42].

The minimum number of vertices (resp., edges) whose deletion yields a bipartite graph from G is called the *vertex bipartiteness* (resp., *edge bipartiteness*) of G and it is denoted $\upsilon_b(G)$ (resp., $\epsilon_b(G)$), see [11]. Let q_n be the smallest eigenvalue of Q_G. In [11], one established the inequalities

$$q_n \leq \upsilon_b(G) \leq \epsilon_b(G). \tag{5}$$

In [42] some important relationships between $\epsilon_b(G)$ and $s_Q(G)$ were found, and it was shown that if $G \ncong P_n$ and $G \ncong C_{2k+1}$ then

$$s_Q(G) \geq 4$$

with equality if and only if G is one of the following graphs: $K_{1,3}$, K_4, two triangles connected by an edge, and C_n with n even.

2. Lower bounds

We now present some new lower bounds for the signless Laplacian spread. The first result gives an upper bound for q_n as function of the vertex bipartiteness, $v_b(G)$, and the independence number of G. It is therefore natural to ask how difficult this parameter is to compute. The *vertex bipartization* problem is to find the minimum number of vertices in a graph whose deletion leaves a subgraph which is bipartite. This problem is NP-hard, even when restricted to graphs of maximum degree 3, see [10]. Actually, this problem has several applications, such as in via minimization in the design of integrated circuits ([10]). Exact algorithms and complexity of different variants have been studied, see [33]. For the parameterized version, where k is fixed and one asks for k vertices whose deletion leaves a bipartite subgraph, an algorithm of complexity $O(3^k \cdot kmn)$ was found in [34]. Similarly, it is NP-hard to compute the edge bipartiteness $\epsilon_b(G)$, even if all degrees are 3, see ([10]). Finally, more general vertex and edge deleting problems were studied in [38], and NP-completeness of a large class of such problems was shown. Recall that an induced subgraph is determined by its vertex set. In fact, deleting some vertices of G together with the edges incident to those vertices we obtain an induced subgraph. A set of vertices that induces an empty subgraph is called an *independent set*. The number of vertices in a maximum independent set of G is called the *independence number* of G and it is denoted by $\alpha(G)$. The problem of finding the independence number of a graph G is also NP-hard, see [14, 24], whereas the spectral bounds can be determined in polynomial time.

Lemma 7. *Let G be a graph with n vertices and independence number $\alpha(G)$. Then*

$$q_n \leq v_b(G) \leq \epsilon_b(G) \leq \frac{(n-\alpha(G))\,(n-\alpha(G)-1)}{2}. \tag{6}$$

Proof. Let $S \subseteq \mathcal{V}(G)$ be an independent set of vertices with cardinality $\alpha = \alpha(G)$ and H be an induced subgraph of G such that $\mathcal{V}(H) = \mathcal{V}(G) \setminus S$. The adjacency matrix of G becomes

$$A_G = \begin{pmatrix} \mathbf{0} & C \\ C^T & A_H \end{pmatrix}$$

where $\mathbf{0}$ is the square zero matrix of order α and the matrix C corresponds to the adjacency relations between the vertices in S and the vertices in H.

Note that the cardinality of the set of edges of H satisfies

$$|\mathcal{E}(H)| \leq \frac{(n-\alpha)(n-\alpha-1)}{2}.$$

The result is obtained since deleting all the edges of H yields a bipartite graph from G. $\square$

Corollary 8. *Let G be an (n,m)-graph with independence number $\alpha = \alpha(G)$. If*

$$n(n-\alpha)(n-\alpha-1) \leq 8m, \tag{7}$$

then

$$s_Q(G) \geq 2\lambda_1 - \upsilon_b(G) \geq \frac{4m}{n} - \upsilon_b(G) \geq 0.$$

Proof. The first inequality in the corollary follows directly from the fact that $q_1 \geq 2\lambda_1$ and Eq. (5). The second inequality follows from below:

$$2\lambda_1 \geq 2\left(\frac{\mathbf{e}^T(A_G)\mathbf{e}}{\mathbf{e}^T\mathbf{e}}\right) = \frac{4m}{n}.$$

As (7) is equivalent to

$$\frac{4m}{n} - \frac{(n-\alpha)(n-\alpha-1)}{2} \geq 0,$$

by Lemma 7

$$\frac{4m}{n} - \upsilon_b(G) \geq \frac{4m}{n} - \frac{(n-\alpha)(n-\alpha-1)}{2} \geq 0,$$

and the desired inequalities follow. $\square$

Remark 9. Note that if $\alpha(G) = n-k$ and as $m \leq \frac{n(n-1)}{2}$ a necessary condition for (7) is $4(n-1) \geq k(k-1)$.

Recall the identity

$$\alpha(G) + \tau(G) = n,$$

where $\tau(G)$ is the vertex cover number of G (that is the size of a minimum vertex cover in a graph G). Replacing in (6) we conclude that

$$\tau(G) \geq \frac{1+\sqrt{1+8\epsilon_b(G)}}{2}.$$

Finding a minimum vertex cover of a general graph is an NP-hard problem. However, for the bipartite graphs, the vertex cover number is equal to the matching number. Therefore, from the previous remark a necessary condition for (7) is, in this case, $4(n-1) \geq \tau(G)(\tau(G)-1)$.

Now, using Theorems 2 and 3 we derive the following results.

Theorem 10. *Let G be a graph of order n with maximum and minimum vertex degree Δ and δ, respectively. If $\Delta - \delta \geq 2$, then*

$$s_Q(G) \geq \left((\Delta-\delta)^2 + 2\Delta + 2\delta\right)^{1/2}.$$

and otherwise (when $\Delta - \delta \leq 1$)

$$s_Q(G) \geq 2\sqrt{\Delta}.$$

Equality holds for $G \cong K_2$.

Proof. Let $Q_G = (q_{ij})$ be the signless Laplacian matrix of G. By Theorem 2

$$s_Q(G) = s(Q_G) \geq \Upsilon$$

where

$$\begin{aligned} \Upsilon &= \max_{i,j} \left((q_{jj}-q_{ii})^2 + 2\sum_{s\neq j} |q_{js}|^2 + 2\sum_{s\neq i} |q_{is}|^2\right)^{1/2} \\ &= \max_{i,j} \left((d_j - d_i)^2 + 2(d_j + d_i)\right)^{1/2}. \end{aligned}$$

In this maximization we may assume (by symmetry) that $d_j \geq d_i$. Moreover, by fixing $d_j - d_i$ to some number $k \in \{0, 1, \ldots, \Delta - \delta\}$, we get

$$\begin{aligned} \Upsilon &= \max_k \max_{d_j - d_i = k} \left((d_j - d_i)^2 + 2(d_j + d_i)\right)^{1/2} \\ &= \max_k \max_{d_j - d_i = k} \left(k^2 + 2(2d_i + k)\right)^{1/2} \\ &= \max_k \left(k^2 + 2(2(\Delta - k) + k)\right)^{1/2} \end{aligned}$$

as $k^2 + 2(2d_i + k)$ is increasing in d_i. So $\Upsilon = \max_k \left(k^2 + 4\Delta - 2k\right)^{1/2}$. But $k^2 + 4\Delta - 2k$ is a convex quadratic polynomial in k so its maximum over $k \in \{0, 1, \ldots, \Delta - \delta\}$ occurs in one of the two endpoints. Therefore

$$\Upsilon = \max\{2\sqrt{\Delta}, \left((\Delta-\delta)^2 + 2(\Delta+\delta)\right)^{1/2}\}$$

which gives the desired result. □

Let $\mathcal{V}(\Delta) = \{v \in \mathcal{V}(G) : d(v) = \Delta\}$ and $\mathcal{V}(\delta) = \{v \in \mathcal{V}(G) : d(v) = \delta\}$.

Theorem 11. *Let G be a graph of order n with maximum and minimum vertex degree Δ and δ, respectively.*

$$s_Q(G) \geq \left((\Delta-\delta)^2 + 2\Delta + 2\delta + 4\right)^{\frac{1}{2}}.$$

We have equality, for instance, when $G \cong K_{1,3}$.

Proof. Let $Q(G) = (q_{ij})$ be the signless Laplacian matrix of G, then Q_G is an $n \times n$ symmetric matrix and by Theorem 3 we derive

$$s_Q(G) = s(Q_G) \geq \Gamma$$

where

$$\Gamma = \max_{i \neq j} \left((q_{ii} - q_{jj})^2 + 2\sum_{s \neq j} |q_{js}|^2 + 2\sum_{s \neq i} |q_{is}|^2 + 4e_{ij} \right)^{1/2},$$

and e_{ij} and f_{ij} are given in Theorem 3.

Let $v_{i_0} \in \mathcal{V}(\Delta)$ and $v_{j_0} \in \mathcal{V}(\delta)$. If $q_{j_0j_0} = q_{i_0i_0}$, then $e_{i_0j_0} = 2f_{i_0j_0}$; otherwise

$$e_{i_0j_0} = \min\left\{ (q_{i_0i_0} - q_{j_0j_0})^2 + 2\left|(q_{i_0i_0} - q_{j_0j_0})^2 - f_{i_0j_0}\right|, \frac{f_{i_0j_0}^2}{(q_{i_0i_0} - q_{j_0j_0})^2} \right\}$$

with

$$f_{i_0j_0} = \left| \sum_{k \neq i_0} |q_{i_0k}|^2 - \sum_{k \neq j_0} |q_{j_0k}|^2 \right| = |d(v_{i_0}) - d(v_{j_0})| = \Delta - \delta.$$

Therefore,

$$e_{i_0j_0} = \min\left\{ (\Delta-\delta)^2 + 2\left|(\Delta-\delta)^2 - (\Delta-\delta)\right|, 1 \right\} = 1.$$

Thus $\Gamma \geq \left((\Delta-\delta)^2 + 2\Delta + 2\delta + 4\right)^{\frac{1}{2}}$ and the result follows.

For $G = K_{1,3}$ it is clear that $s_Q(G) = q_1 = 4$. Moreover, $(\Delta-\delta)^2 + 2\Delta + 2\delta + 4 = 16$. Taking square root, the equality is shown in this case. □

The next Corollary is a direct consequence of the previous theorem.

Let G be a graph with vertex degrees $d_1, d_2, \ldots, d_n$. Let

$$M_1(G) = \sum_{i=1}^{n} d_i^2,$$

be the first Zagreb index [18]. In [30] the following inequality related to the Cauchy-Schwarz inequality is shown. It follows directly from the Lagrange identity (see [36] concerning Lagrange identity and related inequalities).

Lemma 12. [30] *Let* $\mathbf{a} = (a_1, a_2, \ldots, a_n)$ *and* $\mathbf{b} = (b_1, b_2, \ldots, b_n)$ *be two vectors with* $0 < m_1 \leq a_i \leq M_1$ *and* $0 < m_2 \leq b_i \leq M_2$*, for* $i = 1, 2, \ldots, n$*, for some constants* m_1, m_2, M_1 *and* M_2*. Then*

$$\left(\sum_{i=1}^{n} a_i^2\right)\left(\sum_{i=1}^{n} b_i^2\right) - \left(\sum_{i=1}^{n} a_i b_i\right)^2 \leq \frac{n^2}{4}\left(M_1 M_2 - m_1 m_2\right)^2. \qquad (8)$$

By using the above result in what follows, we will obtain a lower bound for the $s_Q(G)$ in terms of $M_1(G)$, n and m.

Theorem 13. *Let* G *be a connected graph with* $n \geq 2$ *vertices. Then*

$$s_Q(G) \geq \frac{2}{n}\sqrt{nM_1(G) - 4m^2 + 2mn}. \qquad (9)$$

Proof. In this proof we use Lemma 12 with $a_i = 1$ and $b_i = q_i$, for $1 \leq i \leq n$. Since $0 < 1 \leq a_i \leq 1$, and $0 < q_n \leq b_i \leq q_1, 1 \leq i \leq n$. Thus $M_1 M_2 = 1q_1$ and $m_1 m_2 = 1q_n$. By Lemma 12

$$\sum_{i=1}^{n} 1 \sum_{i=1}^{n} q_i^2 - \left(\sum_{i=1}^{n} q_i\right)^2 \leq \frac{1}{4} n^2 \left(q_1 - q_n\right)^2$$

then

$$n\left(2m + M_1\left(G\right)\right) - 4m^2 \leq \frac{1}{4} n^2 \left(q_1 - q_n\right)^2.$$

This gives

$$\frac{8m + 4M_1\left(G\right)}{n} - \frac{16m^2}{n^2} \leq s_Q^2(G)$$

and

$$s_Q(G) \geq 2\sqrt{\frac{nM_1(G) - 4m^2 + 2mn}{n^2}}.$$

Thus the result follows. $\square$

3. Lower bounds based on a minmax principle

In this section we introduce a principle for finding several lower bounds for the signless Laplacian spread of a graph.

Let B_n denote the unit ball in $\mathbb{R}^n$, that is, the set of vectors in $\mathbb{R}^n$ such that $\|x\| \leq 1$. The next theorem gives a lower bound on the spread of a real symmetric matrix A. The result is actually known in a slightly different form (see below), but we give a new proof of this inequality, using ideas from minmax theory.

Theorem 14. *Let A be a real symmetric matrix of order n. Then*

$$s(A) \geq 2\|A\mathbf{x} - (\mathbf{x}^T A\mathbf{x})\mathbf{x}\| \quad \text{for all } \mathbf{x} \in B_n. \tag{10}$$

Proof. Lemma 1 in [22] says that $s(A) = 2\min_{t\in\mathbb{R}} \|A - tI_n\|$ where the minimum is over all $t \in \mathbb{R}$ (this follows easily from the spectral theorem). Therefore

$$\begin{aligned} (1/2)s(A) &= \min_{t\in\mathbb{R}} \|A - tI_n\| \\ &= \min_{t\in\mathbb{R}} \max_{\mathbf{x}\in B_n} \|(A - tI_n)\mathbf{x}\| \\ &\geq \max_{\mathbf{x}\in B_n} \min_{t\in\mathbb{R}} \|A\mathbf{x} - t\mathbf{x}\| \\ &= \max_{\mathbf{x}\in B_n} \|A\mathbf{x} - (\mathbf{x}^T A\mathbf{x})\mathbf{x}\|. \end{aligned} \tag{11}$$

The inequality above follows from standard minmax-arguments. In fact, for any function $f = f(\mathbf{x}, t)$ defined on sets X and T, we clearly have $\inf_{t'\in T} f(\mathbf{x}, t') \leq f(\mathbf{x}, t) \leq \sup_{\mathbf{x}'\in X} f(\mathbf{x}', t)$ for all $\mathbf{x} \in X$ and $t \in T$. The desired inequality is then obtained by taking the infimum over t in the last inequality, and then, finally, the supremum over $\mathbf{x}$. The final equality in (11) follows as this is a least-squares problem in one variable t, for given $\mathbf{x} \in B_n$, so geometrically t is chosen so that $t\mathbf{x}$ is the orthogonal projection of $A\mathbf{x}$ onto the line spanned by $\mathbf{x}$. The desired result now follows from (11). □

Below we rewrite the bound in the previous theorem. First, however, note from the proof that the bound in (11) expresses the following: *for any unit vector* $\mathbf{x}$*, twice the distance from* $A\mathbf{x}$ *to the line spanned by* $\mathbf{x}$ *is a lower bound on the spread.* Thus, the bound has a simple geometrical interpretation. This may be useful, in specific situations, in order to find an $\mathbf{x}$ which gives a good lower bound.

Now, a straightforward computation shows that

$$\|A\mathbf{x} - (\mathbf{x}^T A\mathbf{x})\mathbf{x}\|^2 = \mathbf{x}^T A^2\mathbf{x} - (\mathbf{x}^T A\mathbf{x})^2$$

so Theorem 14 says that

$$s(A) \geq 2 \max_{\mathbf{x} \in B_n} \sqrt{\mathbf{x}^T A^2 \mathbf{x} - (\mathbf{x}^T A \mathbf{x})^2}. \tag{12}$$

Therefore this result is actually the result presented in [27, Theorem 4]. In [27] the authors state that this result, in fact, goes back to Bloomfield and Watson in 1975, [4, (5.3)], and it was rediscovered by Styan [37, Theorem 1]. See also [20, section 5.4] and [21].

The result in Theorem 14 may also be reformulated in terms of a nonzero vector $\mathbf{y} = (y_1, y_2, \ldots, y_n)$. Then $\mathbf{x} = (1/\|\mathbf{y}\|)\mathbf{y}$ is a unit vector, and a simple calculation, using (12), gives

$$s(A) \geq 2 \frac{\left(\sum_i y_i^2 \sum_i \tau_i^2 - \left(\sum_i y_i \tau_i\right)^2\right)^{1/2}}{\sum_i y_i^2} \tag{13}$$

where

$$\tau = A\mathbf{y} = (\tau_1, \tau_2, \ldots, \tau_n).$$

Remark 15. From the equality case of Cauchy-Schwarz Theorem, the bound in (13) is equal to zero when the vector τ and $\mathbf{y}$ are a linear combination of the vector $\mathbf{e}$.

We may now obtain different lower bounds on the signless Laplacian spread $s_Q(G)$, for a graph G, by applying Theorem 14 to the signless Laplacian matrix Q_G and choosing some specific unit vector $\mathbf{x}$, or a nonzero vector $\mathbf{y}$, and use (13).

For instance, consider the simple choice $\mathbf{x} = \mathbf{e}_i$, the ith coordinate vector. Then $Q_G \mathbf{e}_i - (\mathbf{e}_i^T Q_G \mathbf{e}_i)\mathbf{e}_i = Q^{(i)} - d_i \mathbf{e}_i$ (where $Q_G^{(i)}$ is the i-th column of Q_G). This gives

$$s_Q \geq 2 \max_i \sqrt{d_i} = 2\sqrt{\Delta}$$

which gives a short proof of the second bound (when $\Delta - \delta \leq 1$) in Theorem 10. Another application of this principle is obtained by using $\mathbf{x}$ as the normalized all ones vector, which gives the following lower bound.

Corollary 16. *Let G be a graph of order n. Then*

$$s_Q(G) \geq \frac{4}{n} \sqrt{n M_1(G) - 4m^2}. \tag{14}$$

Proof. We consider (12) with $A = Q_G$ and $\mathbf{x} = (1/\sqrt{n})\mathbf{e}$ where $\mathbf{e}$ denotes the all ones vector. Then $\mathbf{x}^T A^2 \mathbf{x} = (1/n)\mathbf{e}^T Q_G^2 \mathbf{e}$. Let $\mathbf{d} = (d_1, d_2, \ldots, d_n)$ be the vector whose components are the vertex degrees. So $A_G \mathbf{e} = \mathbf{d}$ and

$$\begin{aligned}
\mathbf{e}^T Q_G^2 \mathbf{e} &= \mathbf{e}^T (D + A_G)^2 \mathbf{e} \\
&= \mathbf{e}^T D^2 \mathbf{e} + \mathbf{e}^T A_G^2 \mathbf{e} + \mathbf{e}^T A_G D \mathbf{e} + \mathbf{e}^T D A_G \mathbf{e} \\
&= M_1(G) + \|A_G \mathbf{e}\|^2 + (A_G \mathbf{e})^T \mathbf{d} + (D\mathbf{e})^T A_G \mathbf{e} \\
&= 4M_1(G).
\end{aligned}$$

Thus (12) gives

$$\begin{aligned}
s_Q(G) &\geq 2\sqrt{4M_1(G)/n - (4m/n)^2} \\
&= (4/n)\sqrt{nM_1(G) - 4m^2},
\end{aligned}$$

and the result follows. ∎

Remark 17. *The lower bounds (14) and (9) are incomparable. Note that for regular graphs (14) is worse than (9) as it is equal to zero and (9) becomes $2\sqrt{r}$, with r vertex degree of the graph. However, for $G = K_{1,n-1}$ (14) is equal to $\frac{4(n-2)\sqrt{n-1}}{n}$ and (9) is $\frac{2(n-2)\sqrt{n-1}}{n}$.*

The following result characterizes the cases which the lower bound in (9) is better than the lower bound in (14) and the proof follows directly by equivalence of the inequalities.

Remark 18. *The lower bound (9) improves the lower bound in (14) if and only if $\frac{2m}{n} \geq \frac{3M_1(G)}{6m+n}$.*

Next, we apply Theorem 14 using the degree vector $\mathbf{d} = (d_1, d_2, \ldots, d_n)$. This gives the following result; it follows directly from (13).

Corollary 19. *Let G be a graph. Then*

$$s_Q(G) \geq 2\frac{\left(\sum_i d_i^2 \sum_i \alpha_i^2 - \left(\sum_i d_i \alpha_i\right)^2\right)^{1/2}}{\sum_i d_i^2} \tag{15}$$

where $\alpha_i = d_i + d_i m_i$, for $i \leq n$, where m_i is the average degree of the vertices that are in $N_G(i)$.

Next, since G is a graph without isolated vertices, we may use (13) with

$$\mathbf{y} = (d_1^{-1}, d_2^{-1}, \ldots, d_n^{-1}),$$

the n-tuple of the reciprocal of the vertex degrees of G.

Corollary 20. *Let G be a graph without isolated vertices. Then*

$$s_Q^2(G) \geq \frac{4}{\left(\sum_i d_i^{-2}\right)^2} \cdot \left(\sum_i d_i^{-2} \sum_j \left(\sum_{v_j v_k \in \mathcal{E}(G)} d_k^{-1} + 1 \right)^2 - \left(\sum_i (\sum_{v_i v_k \in \mathcal{E}(G)} (d_i d_k)^{-1} + d_i^{-1}) \right)^2 \right).$$

Proof. The vector $\tau = (\tau_1, \tau_2, \ldots, \tau_n) = Q\mathbf{y}$ then satisfies

$$\tau_i = 1 + \sum_{v_i v_j \in \mathcal{E}(G)} d_j^{-1}.$$

Moreover,

(1) $\left(\sum_{i=1}^n y_i^2\right)^2 = \left(\sum_{i=1}^n \frac{1}{d_i^2} \right)^2.$

(2) $\left(\sum_{i=1}^n \tau_i^2 \right) = \sum_{i=1}^n \left(1 + \sum_{v_i v_j \in \mathcal{E}(G)} \frac{1}{d_j} \right)^2.$

(3) $\left(\sum_{i=1}^n y_i \tau_i \right)^2 = \left(\sum_{i=1}^n \left(\frac{1}{d_i} + \sum_{v_i v_k \in \mathcal{E}(G)} \frac{1}{d_k d_i} \right) \right)^2.$

Then, considering $\mathbf{x} = (1/\|\mathbf{y}\|)\mathbf{y}$ in (13), the result follows. □

We now establish some other lower bounds on $s_Q(G)$ based on other principles. In what follows the vector of second degrees, denoted by $\mathbf{d}^{(2)}$, is the vector whose components are $d_i m_i$, where m_i is the average degree of the vertices that are in $N_G(i)$.

Theorem 21. *Let G be a graph with vector degrees $\mathbf{d} = (d_1, d_2, \ldots, d_n)$. Moreover, consider $\mathbf{d}^{(2)} = \left(d_1^{(2)}, d_2^{(2)}, \ldots, d_n^{(2)} \right)$ the vector of second degrees of G. Then*

$$s_Q(G) \geq \left| \frac{\sum_{i=1}^n d_i^3 + \sum_{i=1}^n d_i d_i^{(2)}}{M_1(G)} - \Upsilon \right| \qquad (16)$$

with

$$\Upsilon = \min_{\substack{v_p v_q \in \mathcal{E}(G) \\ d(v_q)=\Delta}} \left\{ \frac{\Delta + d_p}{2} - \sqrt{\left(\frac{\Delta + d_p}{2}\right)^2 + 1 - \Delta d_p} \right\}.$$

Note that if G is a bipartite graph then $\Upsilon = 0 = q_n(G)$.

Proof. In [29, Theorem 6] the following lower bound for the spread $s(B)$ of an Hermitian matrix $B = (b_{ij})$ was shown

$$s(B) \geq \max_{p \neq q} \left| \frac{\mathbf{e}^T B^3 \mathbf{e}}{\mathbf{e}^T B^2 \mathbf{e}} - \frac{b_{pp} + b_{qq} \pm \sqrt{(b_{pp} - b_{qq})^2 + 4 |b_{pq}|^2}}{2} \right|.$$

Replacing B by $Q = Q_G$ one has

$$\mathbf{e}^T Q^3 \mathbf{e} = 4 \left(\sum_{i=1}^{n} d_i^3 + \sum_{i=1}^{n} d_i d_i^{(2)} \right).$$

By the proof of Corollary 16 we get

$$\mathbf{e}^T Q^2 \mathbf{e} = 4 M_1 (G).$$

Then

$$\frac{\mathbf{e}^T B^3 \mathbf{e}}{\mathbf{e}^T B^2 \mathbf{e}} = \frac{\mathbf{e}^T Q^3 \mathbf{e}}{\mathbf{e}^T Q^2 \mathbf{e}} = \frac{4 \left(\sum_{i=1}^{n} d_i^3 + \sum_{i=1}^{n} d_i d_i^{(2)} \right)}{4 M_1 (G)}.$$

Moreover, from the proof of Theorem 6 in [29] one sees that

$$\frac{b_{pp} + b_{qq} \pm \sqrt{(b_{pp} - b_{qq})^2 + 4 |b_{pq}|^2}}{2}$$

corresponds to the smallest eigenvalue of the 2×2 submatrix of B,

$$\begin{pmatrix} b_{pp} & b_{pq} \\ b_{pq} & b_{qq} \end{pmatrix},$$

and we will see that the minimum (for the case of Q) corresponds to the smallest eigenvalue of some 2×2 submatrix of Q with the form $\begin{pmatrix} d_p & 1 \\ 1 & d_q \end{pmatrix}$. Two cases must be considered.

(1) The submatrix is $\begin{pmatrix} d_p & 1 \\ 1 & d_q \end{pmatrix}$. By a direct computation, of the mentioned eigenvalue, we obtain

$$\lambda_- = \frac{d_p + d_q}{2} - \sqrt{\left(\frac{d_p + d_q}{2}\right)^2 + 1 - d_p d_q}.$$

Let $x = \frac{d_p+d_q}{2}$ and consider the function

$$f(x) = x - \sqrt{x^2 + \alpha}, x \in (0, \infty),$$

with $\alpha < 0$. From the derivative $f'(x) = 1 - \frac{x}{\sqrt{x^2+\alpha}}$, one easily sees that $f'(x) < 0$, so $f(x)$ is strictly decreasing, thus the minimum

$$\Upsilon = \min_{v_p v_q \in \mathcal{E}(G)} \left\{ \frac{d_p + d_q}{2} - \sqrt{\left(\frac{d_p + d_q}{2}\right)^2 + 1 - d_p d_q} \right\}$$

can not be obtained for small degrees. Recall that the maximum vertex degree is denoted by Δ. We conclude that

$$\Upsilon = \min_{\substack{v_p v_q \in \mathcal{E}(G) \\ d(v_q) = \Delta}} \left\{ \frac{\Delta + d_p}{2} - \sqrt{\left(\frac{\Delta + d_p}{2}\right)^2 + 1 - \Delta d_p} \right\}.$$

(2) The submatrix is $\begin{pmatrix} d_p & 0 \\ 0 & d_q \end{pmatrix}$.

It is clear that its smaller eigenvalue is

$$\min\{d_p, d_q\},$$

thus $\Upsilon = \delta$ is the minimum vertex degree of G. We recall the above function $f(x) = x - \sqrt{x^2 + \alpha}$, $x \in (0, \infty)$ with $\alpha < 0$. If $x = \delta$, then $\delta \leq \frac{d_p+d_q}{2}$, implies

$$f(\delta) = \delta - \sqrt{\delta^2 + \alpha} \geq f\left(\frac{d_p + d_q}{2}\right) = \frac{d_p + d_q}{2} - \sqrt{\left(\frac{d_p + d_q}{2}\right)^2 + \alpha}.$$

As the constant α in function f equals the negative number $\alpha = 1 - d_p d_q$, we have

$$f(\delta) = \delta - \sqrt{\delta^2 + \alpha} \geq \frac{d_p + d_q}{2} - \sqrt{\left(\frac{d_p + d_q}{2}\right)^2 + 1 - d_p d_q}.$$

Moreover, as

$$\delta \geq \delta - \sqrt{\delta^2 + \alpha} \geq \frac{d_p + d_q}{2} - \sqrt{\left(\frac{d_p + d_q}{2}\right)^2 + 1 - d_p d_q},$$

the result follows. $\square$

4. Upper bounds

In [6], using the Mirsky's upper bound mentioned above, it was shown that for a graph G with $n \geq 5$ vertices and $m \geq 1$ edges, the following inequality holds

$$s_L(G) \leq \sqrt{2M_1(G) + 4m - \frac{8m^2}{n-1}}.$$

Here equality holds if and only if G is one of the graphs K_n, $G(\frac{n}{4}, \frac{n}{4})$, $K_1 \vee 2K_{\frac{n-1}{2}}$, $\overline{K}_{\frac{n}{3}} \vee 2K_{\frac{n}{3}}$, $K_1 \cup K_{\frac{n-1}{2}, \frac{n-1}{2}}$, $K_{\frac{n}{3}} \cup K_{\frac{n}{3}, \frac{n}{3}}$. The graph $G(r,s)$ is the graph obtained by joining each vertex of the subgraph $\overline{K}_s$ of $K_r \vee \overline{K}_s$ to all the vertices of $\overline{K}_s$ of another copy of $K_r \vee \overline{K}_s$. Here $G \vee G'$ is the usual join operation between two graphs G and G'.

Theorem 22. *Let G be an (n,m)-graph. Then*

$$s_Q(G) \leq \sqrt{2\left(\sum_{i=1}^{n} d_i^2 + 2m\right) - \frac{8m^2}{n}} = \sqrt{2M_1(G) + 4m - \frac{8m^2}{n}}. \quad (17)$$

The equality is attained if and only if $G \simeq K_{\frac{n}{2}, \frac{n}{2}}$.

Proof. Since $Q = Q(G)$ is a normal matrix, by applying Theorem 1 to Q we obtain

$$s_Q(G) = s(Q) \leq \sqrt{2\,\|Q\|_F^2 - \frac{2}{n}(\operatorname{tr} Q)^2}$$

with equality if and only if the eigenvalues $q_1, q_2, \ldots, q_n$ satisfying the following condition

$$(*) \quad q_2 = q_3 = \cdots = q_{n-1} = \frac{q_1 + q_n}{2}.$$

As $\|Q\|_F^2 = M_1(G) + 2m$ and $\operatorname{tr} Q = 2m$, the result follows. If condition $(*)$ holds then

$$\operatorname{tr} Q = nq_2$$

so

$$q_2 = \frac{2m}{n} = \frac{1}{2}\frac{\mathbf{e}^T Q\,(G)\,\mathbf{e}}{\mathbf{e}^T\mathbf{e}} \leq \frac{1}{2}q_1,$$

by [35, Lemma 1.1]. Then

$$q_1 + q_n = 2q_2 \leq q_1$$

so $q_n = 0$ and $q_2 = \frac{1}{2}q_1$. This gives

$$q_1 = 2q_2 = \frac{4m}{n}.$$

Thus, G is a regular bipartite graph and the statement holds. Conversely, if $G \simeq K_{\frac{n}{2},\frac{n}{2}}$, by a standard verification, the inequality in Theorem 22 holds with equality. ∎

Corollary 23. *Let G_k be a k-regular graph with n vertices. Then*

$$s_Q(G) \leq \sqrt{2nk}.$$

Here equality is attained if and only if $G \simeq K_{\frac{n}{2},\frac{n}{2}}$.

Proof. We get $M_1(G_k) = nk^2$ and $m = \frac{nk}{2}$. Thus,

$$2M_1(G_k) + 4m - \frac{8m^2}{n} = 2nk^2 + 4\frac{nk}{2} - \frac{8}{n}\left(\frac{nk}{2}\right)^2 = 2nk^2 + 2nk - 2nk^2 = 2nk.$$

By Theorem 22, the result now follows. If $G \simeq K_{\frac{n}{2},\frac{n}{2}}$, then G is a regular bipartite graph with $k = \frac{n}{2}$, so $\sqrt{2nk} = \sqrt{2n\frac{n}{2}} = n = \mu_1(K_{\frac{n}{2},\frac{n}{2}}) = s_Q(K_{\frac{n}{2},\frac{n}{2}})$. ∎

Corollary 24. *Let G be an (n,m)-graph. Then*

$$s_Q(G) \leq \sqrt{2m(\frac{2m}{n-1} + \frac{n-2}{n-1}\Delta + (\Delta-\delta)(1-\frac{\Delta}{n-1})) + 4m - \frac{8m^2}{n}}. \quad (18)$$

The equality is attained if and only if $G \simeq K_{\frac{n}{2},\frac{n}{2}}$.

Proof. In [7] it was shown that

$$M_1(G) \leq m(\frac{2m}{n-1} + \frac{n-2}{n-1}\Delta + (\Delta-\delta)(1-\frac{\Delta}{n-1})) \quad (19)$$

with equality if and only if G is either a star, a regular graph or a complete graph $K_{\Delta+1}$ with $n-\Delta-1$ isolated vertices. Replacing $M_1(G)$ in (17) by its upper bound in (19) the result follows. Equality holds in (18) if and only if equality holds in both (17) and (19), or equivalently $G \simeq K_{\frac{n}{2},\frac{n}{2}}$. □

5. Comparison of bounds

This section deals with a comparison of some of the bounds presented in this work. We firstly compare the bound in Theorem 11 with the lower bound for $s_Q(G)$ (depending on same parameters) found in [26, Corollary 2.3]:

$$s_Q(G) \geq \frac{1}{n-1}\left((n\Delta)^2 + 8(m-\Delta)(2m-n\Delta)\right)^{\frac{1}{2}}.$$

Let $L_1(G)$ and $L_2(G)$ denote the bound from Theorem 11 and [26], respectively, so

$$\begin{aligned} L_1(G) &= \left((\Delta-\delta)^2 + 2\Delta + 2\delta + 4\right)^{\frac{1}{2}}, \\ L_2(G) &= \tfrac{1}{n-1}\left((n\Delta)^2 + 8(m-\Delta)(2m-n\Delta)\right)^{\frac{1}{2}}. \end{aligned}$$

Observe that $L_1(G)$ only depends on the minimum and maximum degrees, not n and m. Let $\bar{d} = (1/n)\sum_{i=1}^n d_i = 2m/n$ denote the average degree in G. So

$$\begin{aligned} L_2(G) &= \tfrac{n}{n-1}\left(\Delta^2 + \tfrac{8(m-\Delta)(2m-n\Delta)}{n^2}\right)^{\frac{1}{2}} \\ &= \tfrac{n}{n-1}\left(\Delta^2 + (4\bar{d} - \tfrac{8\Delta}{n})(\bar{d}-\Delta)\right)^{\frac{1}{2}} \end{aligned}$$

which shows that $L_2(G)$ is determined by the maximum and average degree as well as n. Here $\bar{d}-\Delta \leq 0$, and $\bar{d}-\Delta = 0$ precisely when G is regular.

The next result relates the two lower bounds as a function of certain graph properties.

Remark 25. *Let G be a an (n,m)-graph with $n > 2$.*

(i) *Assume G is a k-regular graph. Then $L_1(G) = 2\sqrt{k+1}$ and $L_2(G) = \frac{n}{n-1}k$. Therefore, $L_2(G) > L_1(G)$ except when $k \leq 3$ (and n arbitrary) or $k = 4$ and $n \geq 10$.*

(ii) *Assume G is connected and contains a pendant vertex. Then $L_2(G) \leq \frac{n}{n-1}\Delta$ and $L_1(G) = \sqrt{\Delta^2+7}$. In particular, $L_2(G) < L_1(G)$ holds if $\frac{2n-1}{(n-1)^2}\Delta^2 < 7$.*

In fact, for (i) consider the case when G is regular, say of degree k. The two expressions follow from the calculation above as $\bar{d} = \delta = \Delta = k$. Then $L_2(G) \leq L_1(G)$ gives $\frac{n}{n-1}k \leq 2\sqrt{k+1}$, or $1 - \frac{1}{n} \geq \frac{k}{2\sqrt{k+1}}$. Here the right hand side is greater than 1 precisely when $k \geq 5$, and the conclusion then follows.

(ii) Since there is a pendant vertex, $\delta = 1$. This gives

$$L_1(G) = \sqrt{(\Delta-1)^2 + 2\Delta + 2 + 4} = \sqrt{\Delta^2+7}.$$

We have $\Delta > \delta = 1$, for if $\Delta = 1$, G would be a perfect matching, contradicting that G is connected and $n > 2$. Therefore $\bar{d} - \Delta < 0$. Moreover, as G is connected, $m \geq n-1 \geq \Delta$. So $m \geq \Delta$, and using that $2m = \sum_i d_i$, we easily derive $4\bar{d} \geq 8\Delta/n$. Therefore

$$L_2(G) = \frac{n}{n-1}\left(\Delta^2 + (4\bar{d} - \frac{8\Delta}{n})(\bar{d}-\Delta)\right)^{\frac{1}{2}} \leq \frac{n}{n-1}\left(\Delta^2\right)^{\frac{1}{2}} = \frac{n}{n-1}\Delta.$$

Therefore, if $\frac{n}{n-1}\Delta < \sqrt{\Delta^2+7}$, then $L_2(G) < L_1(G)$. The last statement follows from this.

Consider again our lower bound on the signless Laplacian spread $s_Q(G)$

$$\eta(G) := 2\max_{\mathbf{x}\in B_n} \|Q\mathbf{x} - (\mathbf{x}^T Q\mathbf{x})\mathbf{x}\|. \tag{20}$$

In the proof we obtained the bound by some calculations in which a single inequality was involved, namely when we used that "minmax" is at least as large as "maxmin", for the function involved. Unfortunately, we cannot show that equality holds here. The reason for this is basically that $\|(Q - tI_n)\mathbf{x}\|$ is not a concave function of $\mathbf{x}$ and, also, B_n is not a convex set, so general minmax theorems may not be applied to our situation.

However, it is interesting to explore further the quality of the best bound one gets from the minmax principle. To do so, consider the function

$$f(\mathbf{x}) = 2\|Q\mathbf{x} - (\mathbf{x}^T Q\mathbf{x})\mathbf{x}\|$$

so that $\eta(G) = \max_{\mathbf{x}\in B_n} f(\mathbf{x})$. Note that f is a complicated function, obtained from a multivariate polynomial of degree six (by taking the square root, although that can be removed for the maximization). We consider an extremely simple approach to approximately maximize f over the unit ball; we perform a few iterations K of the following gradient method with a step length $s > 0$:

Algorithm: Simple gradient search.

1. Let $\mathbf{x} = (1/\sqrt{n})\mathbf{e}$, and $\eta = f(\mathbf{x})$.
2. for $k = 1, 2, \ldots, K$
   (i) compute a numerical approximation $\mathbf{g}$ to the gradient of f at $\mathbf{x}$,
   (ii) gradient step and projection: let $\mathbf{y} := \mathbf{x} + s \cdot \mathbf{g}$ and $\mathbf{y} := (1/\|\mathbf{y}\|)\mathbf{y}$,
   (iii) update: $\eta := \max\{\eta, f(\mathbf{y})\}$ and $\mathbf{x} := \mathbf{y}$.
3. Output η.

In each iteration, we make a step in the direction of the (numerical) gradient, even if the new function value could be less. Thus we avoid line search. The disadvantage is that we may not approximate a local maximum so well, but the advantage is that we can escape a local maximum and go towards another with higher function value. The procedure is very simple, and heuristic, and we typically only perform a few iterations K (around 10 or 20). We have used constant step length s, but also variable step length (being a decreasing function of the iteration number).

In the table below we give some computational results, for 5 random, connected graphs, showing all previous lower bounds we have discussed and the new bound η. The notation in the table is the following:

$$
\begin{aligned}
liu_{2.2} &= [26], \text{Theorem 2.2} \\
liu_{2.3} &= [26], \text{Corollary 2.3} \\
meg_1 &= \text{bound in Theorem 13} \\
meg_2 &= \text{bound in Theorem 11} \\
Ncon &= \text{bound in Corollary 16} \\
Z1 &= \text{from Theorem 14 (minmax principle), using inverse of degrees} \\
Z2 &= \text{from Theorem 14, using vector of } d_i^{-3} \\
\eta &= \text{best bound from simple gradient method for the function } \eta(\mathbf{x}), \text{ 10 iterations} \\
spread &= \text{exact } s_Q \text{ spread.}
\end{aligned}
$$

n	m	Δ	δ	$liu_{2.2}$	$liu_{2.3}$	meg_1	meg_2	$Ncon$	$Z1$	$Z2$	η	$spread$
40	634	36	27	32.60	28.68	11.91	14.53	7.76	11.76	19.31	38.39	39.19
40	519	32	20	26.99	21.38	11.81	15.87	11.96	17.75	26.68	31.07	36.03
40	322	23	9	17.07	11.06	9.97	16.25	11.83	17.79	23.16	25.14	26.34
40	273	19	9	14.42	9.69	8.98	12.65	10.22	14.87	18.41	20.48	22.50
40	346	22	12	18.01	13.74	9.66	13.11	9.81	15.00	21.82	23.94	26.33

For the last example above we next show the value of η during the 10 iteration of the gradient search algorithm, and we see that that maximum, in this case, was found in iteration 4:

iteration	1	2	3	4	5	6	7	8	9	10
$f(\mathbf{x})$	9.80	21.77	23.41	23.94	22.81	18.77	22.34	17.32	23.20	19.34

These, and similar, experiments clearly show that $\eta(G)$ is a *very good* lower bound on the signless Laplacian spread $s_Q(G)$. Although the exact computation of $\eta(G)$ may be hard, we see that a simple gradient algorithm finds very good approximations, and lower bounds on $s_Q(G)$, in a few iterations. Of, course, the result of such an algorithm is not an analytical bound in terms of natural graph parameters. But every bound needs to be computed, and, in practice, its computational effort should always be compared to the work of using an eigenvalue algorithm for computing the largest and smallest eigenvalue of Q, and finding $s_Q(G)$ in that way.

Finally, we remark that it is possible to use the results above to find such an analytical bound which is quite good: compute the exact gradient (of $f(\mathbf{x})^2$) at the constant vector and make one iteration in the gradient algorithm; let $\hat{\mathbf{x}}$ be the obtained unit vector, and compute the bound $f(\hat{\mathbf{x}})$. We leave this computation to the interested reader.

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