Bounds on the Q-spread of a graph

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Abstract

The spread $s(M)$ of an $n \times n$ complex matrix M is $s(M) = max_{ij}|\lambda_i - \lambda_j|$, where the maximum is taken over all pairs of eigenvalues of M, $\lambda_i, 1 \leq i \leq n$, [9] and [11]. Based on this concept, Gregory *et al.* [7] determined some bounds for the spread of the adjacency matrix $A(G)$ of a simple graph G and made a conjecture regarding the graph on n vertices yielding the maximum value of the spread of the corresponding adjacency matrix. The signless Laplacian matrix of a graph G, $Q(G) = D(G) + A(G)$, where $D(G)$ is the diagonal matrix of degrees of G and $A(G)$ is its adjacency matrix, has been recently studied, [4], [5]. The main goal of this paper is to determine some bounds on $s(Q(G))$. We prove that, for any graph on $n \geq 5$ vertices, $2 \leq s(Q(G)) \leq 2n - 4$, and we characterize the equality cases in both bounds. Further, we prove that for any connected graph G with $n \geq 5$ vertices, $s(Q(G)) < 2n - 4$. We conjecture that, for $n \geq 5$, $s_Q(G) \leq \sqrt{4n^2 - 20n + 33}$ and that, in this case, the upper bound is attained if, and only if, G is a certain path-complete graph.

Key words:
spectrum, signless Laplacian matrix, spread, path complete graph

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1 Introduction

For an $n \times n$ complex matrix M, the spread $s(M)$ of M is defined as the diameter of its spectrum, that is, $s(M) = max_{i,j}|\lambda_i - \lambda_j|$, where the maximum is taken over all pairs of eigenvalues of M. There are several results concerning the spread of a matrix, see for example [10], [9], [11], [1] and [14]. Let $G = (V, E)$ be a simple, undirected graph of order n with adjacency matrix A and the vertex degrees $\Delta = d_G(v_1) \geq d_G(v_2) \geq \cdots \geq d_G(v_n) = \delta$. Gregory *et al.*[7] have determined bounds for the spread of the adjacency matrix of a simple graph, see [7] for further details.

Let $D(G)$ be the diagonal matrix of vertex degrees of G and $L(G) = D(G) - A(G)$, the Laplacian matrix of G. Since the minimum eigenvalue of $L(G)$ is zero, the spread of $L(G)$ is equal to the spectral radius of $L(G)$, a parameter that has received much recent attention. Related to the Laplacian matrix is the so-called signless Laplacian matrix of a graph G, $Q(G) = D(G) + A(G)$, which has recently been studied, [4], [5]. For a graph G on n vertices, we denote the spectrum of $Q(G)$ by $Spec(Q(G)) = (q_1, \ldots, q_{n-1}, q_n)$, where $q_1 \geq \ldots \geq q_{n-1} \geq q_n$. It is readily seen that $Q(G)$ is positive semidefinite, so that $q_i \geq 0$, $i = 1, \ldots, n$, and Cvetković *et al.* [5] proved that $q_n(G) = 0$ if and only if G is a bipartite graph. In this case, the study of the spread of $Q(G)$, which we refer to as the Q-spread, and denote by $s_Q(G)$, is reduced to the study of $q_1(G)$. In this paper, we are interested in determining upper and lower bounds on $s_Q(G)$ in the case that G is not constrained to be a bipartite graph.

This paper is organized as follows. In the next section, we determine upper and lower bounds on the Q-spread among all simple graphs on a given number of vertices. Section 3 is dedicated to the special case of the path complete graphs $PC_{n,p,t}$ when $t = 1$. We determine the spectrum of all $PC_{n,p,1}$-graphs and we prove that $PC_{n,1,1}$ maximizes the Q-spread over the class of graphs of the form $G = PC_{n,p,1}$. For another results to the path complete graphs see [8], [12], [2]. The paper ends with a conjecture that $PC_{n,1,1}$ maximizes $s_Q(G)$ over the class of connected graphs on n vertices.

2 Bounds for the Q-spread of a graph

In this section we find sharp lower and upper bounds for $s_Q(G)$ where G is a simple graph with at least one edge. The bulk of the work below is in dealing with the case that G is connected, and as will be seen in Section 3, we believe that the upper bound for connected graphs given here can be improved.

It is straightforward to see that for any graph G we have $s_Q(G) \geq 0$, with equality holding if and only if G has no edges. Our first result deals with the case that G has at least one edge.

Proposition 1 *Suppose that G is a graph on n vertices with at least one edge. Then $s_Q(G) \geq 2$, with equality holding if and only if G consists of a union of independent edges and possibly some isolated vertices.*

PROOF. Let G have minimum degree δ and maximum degree Δ. We have $q_1(G) \geq \Delta$ and $q_n(G) \leq \delta$, so that $s_Q(G) \geq \Delta - \delta$. If $\Delta - \delta \geq 3$, then certainly $s_Q(G) > 2$, so suppose now that $\Delta \leq \delta + 2$. Note that if $\Delta = \delta$, so that G is regular, then we find readily that $q_1(G) \geq \delta + 1, q_n(G) \leq \delta - 1$, so that $s_Q(G) \geq 2$. In the regular case, we see that $s_Q(G) = 2$ only if $q_1(G) = \delta + 1$, which in turn yields that each connected component of G consists of a single edge. Henceforth, we suppose that G is not regular.

Observe that if $\delta = 0$, then since G has at least one edge, $q_1(G) \geq 2$, yielding the desired inequality; the equality case then follows from the fact that $q_1(G) = 2$ if and only if each connected component of G on at least two vertices consists of a single edge. Henceforth, we assume that $\delta \geq 1$.

Note that any vertex of degree δ is adjacent to a vertex of degree $\delta + i$ for some $i = 0, 1, 2$ (the latter case occurring only if $\Delta = \delta + 2$). Hence for some such i, $Q(G)$ contains a principal 2×2 submatrix that is permutationally similar to $T = \begin{bmatrix} \delta + i & 1 \\ 1 & \delta \end{bmatrix}$. It now follows from interlacing that $q_n(G)$ is bounded above by the smallest eigenvalue of T, which is $\frac{2\delta + i - \sqrt{i^2+4}}{2}$.

Note also that, when the vertices of G are suitably labelled, there is a principal submatrix of Q of order $\Delta + 1$ that is entrywise greater than or equal to the matrix $S = \begin{bmatrix} \Delta & 1 & 1 & \ldots & 1 \\ 1 & \delta & 0 & \ldots & 0 \\ 1 & 0 & \delta & \ldots & 0 \\ \vdots & & & \ddots & \vdots \\ 1 & 0 & \ldots & 0 & \delta \end{bmatrix}$. Hence we find that $q_1(G)$ is bounded below by the Perron value of S, which is readily seen to be $\frac{\Delta + \delta + \sqrt{(\Delta - \delta)^2 + 4\Delta}}{2}$.

From the above considerations, we find that $s_Q(G) \geq \frac{\Delta + \delta + \sqrt{(\Delta - \delta)^2 + 4\Delta}}{2} - \frac{2\delta + i - \sqrt{i^2+4}}{2} = \frac{\Delta - \delta - i + \sqrt{(\Delta - \delta)^2 + 4\Delta} + \sqrt{i^2+4}}{2}$. Thus for the case that $\Delta = \delta + 2$, we have that for some $i = 0, 1, 2$, $s_Q(G) \geq \frac{2 - i + \sqrt{12 + 4\delta} + \sqrt{i^2+4}}{2}$; since $\delta \geq 1$, we thus find that $s_Q(G) \geq 3$. For the case that $\Delta = \delta + 1$, we have that for some $i = 0, 1$, $s_Q(G) \geq \frac{1 - i + \sqrt{5 + 4\delta} + \sqrt{i^2+4}}{2}$; since $\delta \geq 1$, we have $s_Q(G) > \frac{5}{2}$.

The conclusion now follows. ■

Proposition 2 *For any connected bipartite graph G with n vertices,*

$$s_Q(P_n) = 2 + 2\cos\frac{\pi}{n} \leq s_Q(G).$$

PROOF. As noted in Section 1 for any bipartite graph, the Q-spread coincides with $q_1(G)$ (or equivalently, the Laplacian spectral radius of G). According to Yan [13], for any bipartite graph G, $2 + 2\cos\frac{\pi}{n} \leq q_1(G)$, and the path P_n is the unique graph such that $q_1(P_n)$ attains this lower bound. ■

Remark 1: Based on a number of computational tests using the AutoGraphiX System [3], Cvetković *et al.* [6] conjectured the following result concerning lower and upper bounds for $s_Q(G)$.

Conjecture 3 *Fix $n \geq 6$. Of all connected graphs on n vertices, $s_Q(G)$ is maximized by $K_{n-1} + e$, the graph formed by adding a pendant edge to K_{n-1}. Further, of all connected graphs on n vertices, $s_Q(G)$ is minimized by the path P_n and, in the case that n is odd, by the cycle C_n.*

Next, we turn our attention to finding an upper bound on the Q-spread for connected graphs.

Lemma 4 *Suppose that G is a connected graph on n vertices with maximum degree at most $n-2$. Then $s_Q(G) \leq 2n-4$, and equality holds if and only if $n = 4$ and $G = C_4$.*

PROOF. Let the maximum degree of G be Δ. We have $q_1(G) \leq 2\Delta \leq 2n-4$, and so certainly $s_Q(G) \leq 2n-4$. Suppose now that $s_Q(G) = 2n-4$; then necessarily G is regular of degree $n-2$, so that $Q(G) = (n-2)I + A(G)$. Further, $q_n(G) = 0$, so that $A(G)$ has $-(n-2)$ as an eigenvalue. Hence, G must be bipartite, in addition to being regular of degree $n-2$. It now follows that each of the partite sets in the bipartition of V has cardinality at most 2, so that $n \leq 4$. It is straightforward to determine now that $n = 4$ and $G = C_4$. ■

Our main result of this section, the upper bound on the Q-spread for connected graphs given by Theorem 12, requires a number of technical lemmas, which follow. Henceforth we let J denote an all ones matrix, $\mathbf{1}$ denote an all ones vector, $\mathbf{0}$ denote a zero vector, and I denote an identity matrix; orders for each will be clear from the context.

Lemma 5 *Suppose that G is a graph on n vertices such that $q_1(G) > 2n-4$. Then G has maximum degree $n-1$. If G has, say, k vertices of degree $n-1$, then $q_1(G) \le \frac{1}{2}(3n-6+\sqrt{(n-2)^2+8k})$. The equality holds if and only if G also has $n-k$ vertices of degree $n-k-2$.*

PROOF. Let Δ be the maximum degree of G. Since $2\Delta \ge q_1(G) > 2n-4$, we see that $\Delta > n-2$. Hence we must have $\Delta = n-1$. Suppose that G has k vertices of degree $n-1$. Then $Q(G)$ can be written as

$$Q(G) = \left[\begin{array}{c|c} (n-2)I+J & J \\ \hline J & B \end{array}\right],$$

where $B = kI + Q(H)$, and H is the subgraph of G induced by the vertices of degree less than $n-1$. Note that $(B\mathbf{1})_i = k + 2d_H(v_i)$. Since $d_H(v_i) \le n-2-k$, $B\mathbf{1} \le (k+2(n-2-k))\mathbf{1} = (2n-k-4)\mathbf{1}$, where $\mathbf{1}$ denotes the all ones vector. It follows that $q_1(G)$ is bounded above by the Perron value of the 2×2 matrix

$$M = \begin{bmatrix} n-2+k & n-k \\ k & 2n-k-4 \end{bmatrix}.$$

A computation shows that the Perron value of M is given by $\frac{1}{2}(3n-6+\sqrt{(n-2)^2+8k})$.

Observe that $B\mathbf{1} = k+2(n-2-k)$ if and only if the remaining $n-k$ vertices of G have the same degree $n-k-2$. So, the unique graph G on k vertices of degree $n-1$ that has maximum q_1 also has $n-k$ vertices of degree $n-k-2$ and the conclusion follows. ■

Let O_{n-k} denote the empty graph on $n-k$ vertices; we define the graph $G_R(n,k)$ as the join of K_k and O_{n-k}, i.e., $G_R(n,k) = K_k \nabla O_{n-k}$. Let $\mathcal{M}_n$ be the set of all semi-definite positive matrices of order n. Let M_1 and $M_2 \in \mathcal{M}_n$. We call that M_2 is bounded below by M_1 in a positive semi-definite ordering if $x^T M_1 x \le x^T M_2 x$, for all $x \in R^n$, $x \ne 0$.

Lemma 6 *Let $G \ne K_n$ be a graph on n vertices with k vertices of degree $n-1$. Then $q_n(G) \ge \frac{1}{2}(n+2k-2-\sqrt{(n+2k-2)^2-8k(k-1)})$.*

PROOF. Note that with a suitable numbering of the vertices of G, $Q(G)-$

$Q(G_R(n,k))$ is a positive semidefinite matrix, where $Q(G_R(n,k))$ is given by

$$Q(G_R(n,k)) = \left[\begin{array}{c|c} (n-2)I+J & J \\ \hline J & kI \end{array}\right],$$

and where the diagonal blocks in the partitioning are of orders k and $n-k$, respectively. Consequently, $q_n(Q(G)) \geq q_n(Q(G_R(n,k)))$.

For each $i = 1, \ldots, n$, let e_i denote the i-th standard unit basis vector. We find that for each $j = 2, \ldots, k, e_1 - e_j$ is an eigenvector for $Q(G_R(n,k))$ corresponding to eigenvalue $n-2$, while for each $j = k+2, \ldots, n, e_{k+1} - e_j$ is an eigenvector for $Q(G_R(n,k))$ corresponding to eigenvalue k. Consequently, we see that $Q(G_R(n,k))$ has $n-2$ as an eigenvalue of multiplicity at least $k-1$, and k as an eigenvalue of multiplicity at least $n-k-1$. Further, since $Q(G_R(n,k))$ has an orthogonal basis of eigenvectors, it follows that there are remaining eigenvectors of $Q(G_R(n,k))$ of the form $\begin{bmatrix} \alpha\mathbf{1} \\ \beta\mathbf{1} \end{bmatrix}$. It follows that the remaining eigenvalues of $Q(G_R(n,k))$ coincide with those of the 2×2 matrix

$$S = \begin{bmatrix} n-2+k & n-k \\ k & k \end{bmatrix}.$$

The eigenvalues of S are readily seen to be

$$\frac{1}{2}(n+2k-2 \pm \sqrt{(n+2k-2)^2 - 8k(k-1)}),$$

and thus we find that $q_n(G) \geq \min\{k, n-2, \frac{1}{2}(n+2k-2-\sqrt{(n+2k-2)^2-8k(k-1)})\}$. Since $k \geq \frac{1}{2}(n+2k-2-\sqrt{(n+2k-2)^2-8k(k-1)})$, and $n-2 \geq \frac{1}{2}(n+2k-2-\sqrt{(n+2k-2)^2-8k(k-1)}$ the conclusion follows.■

Corollary 7 *$G_R(n,k)$ is the unique connected graph that minimizes q_n among all non-complete graphs on n vertices with at least k vertices of degree $n-1$.*

PROOF. It suffices to show that $q_n(G_R(n,k)) < q_n(G_R(n,k) \cup e)$ when we add an edge e between two vertices of degree k of $G_R(n,k)$. With a suitable labelling of the vertices, we have

$$Q(G_R(n,k) \cup e) = \left[\begin{array}{c|c|cc} (n-2)I+J & J & \multicolumn{2}{c}{J} \\ \hline J & kI & \multicolumn{2}{c}{O} \\ \hline & & k+1 & 1 \\ J & O & & \\ & & 1 & k+1 \end{array}\right]$$

As in Lemma 6, we find that the eigenvalues of $Q(G_R(n,k) \cup e)$ are $n-2$ (with multiplicity $k-1$), k (with multiplicity $n-k-2$), as well as the eigenvalues of the matrix

$$S = \begin{bmatrix} n-2+k & n-2-k & 2 \\ k & k & 0 \\ k & 0 & k+2 \end{bmatrix}.$$

According to Lemma 6, the least eigenvalue x of $Q(G_R(n,k))$ is $x = \frac{1}{2}(n + 2k - 2 - \sqrt{(n+2k-2)^2 - 8k(k-1)})$. So, if we show that $S - xI$ is positive definite, the result will follow. We have

$$S - xI = \begin{bmatrix} n-2+k-x & n-2-k & 2 \\ k & k-x & 0 \\ k & 0 & k+2-x \end{bmatrix},$$

so that $\det(S - xI) =$
$(k+2-x)[(n-2+k-x)(k-x) - k(n-2-k)] + k(-2)(k-x)$
$= 4k > 0.$
Since $k - x$ and $n - 2 + k - x$ are positive the result follows. ■

The following result was established by generating all graphs satisfying the hypotheses and then verifying the inequality on the Q-spread.

Lemma 8 *Let G be a graph on $n = 5, 6,$ or 7 vertices, with $k \geq 3$ vertices of degree $n-1$. Then, $s_Q(G) < 2n-4$.*

Lemma 9 *Suppose the G is a graph on $n \geq 8$ vertices, with $k \geq 3$ vertices of degree $n-1$. Then $s_Q(G) < 2n-4$.*

PROOF. If $k = n$, then $G = K_n$ and $s_Q(K_n) = n < 2n-4$ for $n \geq 8$. Now we consider two cases. In the first case, suppose that $q_1(G) > 2n-4$. From Lemma

5 we find that $q_1(G) \leq \frac{1}{2}(3n-6+\sqrt{(n-2)^2+8k})$, while from Lemma 6 we have $q_n(G) \geq \frac{1}{2}(n+2k-2-\sqrt{(n+2k-2)^2-8k(k-1)})$. Hence, $s_Q(G) \leq \frac{1}{2}(3n-6+\sqrt{(n-2)^2+8k}) - \frac{1}{2}(n+2k-2-\sqrt{(n+2k-2)^2-8k(k-1)}) = \frac{1}{2}(2n-2k-4+\sqrt{(n-2)^2+8k}+\sqrt{(n+2k-2)^2-8k(k-1)})$. Note that $\sqrt{(n-2)^2+8k} < n-2+\frac{4k}{n-2}$ and that $\sqrt{(n+2k-2)^2-8k(k-1)} < n+2k-2-\frac{4k(k-1)}{n+2k-2}$, so it follows that $s_Q(G) < n-k-2+\frac{n-2+\frac{4k}{n-2}}{2}+\frac{n+2k-2-\frac{4k(k-1)}{n+2k-2}}{2} = 2n-4+2k\left(\frac{1}{n-2}-\frac{k-1}{n+2k-2}\right)$. Since $k \geq 3$ and $n \geq 8$, we have $\frac{1}{n-2} \leq \frac{k-1}{n+2k-2}$, and the conclusion follows.

In the second case, suppose $q_1(G) \leq 2n-4$. If $q_1(G) < 2n-4$, we have the result. Now, consider $q_1(G) = 2n-4$. Suppose, to the contrary, that $s_Q(G) = 2n-4$. In this case q_n must be zero. From [5] G is a bipartite graph and hence the spectrum of the signless Laplacian and Laplacian are the same. So, $q_1(G) \leq n < 2n-4$. We thus conclude that $s_Q(G) < 2n-4$. ■

Lemma 10 *Suppose that G is a graph on $n \geq 7$ vertices with $k = 1$ or 2 vertices of degree $n-1$, and no vertices of degree $n-2$. Then $q_1(G) < 2n-4$.*

PROOF. We may write $Q(G)$ as

$$Q(G) = \left[\begin{array}{c|c} (n-2)I+J & J \\ \hline J & B \end{array}\right],$$

where $B = kI+Q(H)$, and H is the subgraph of G induced by the vertices of degree less than $n-2$. Note that $B\mathbf{1} \leq (k+2(n-3-k))\mathbf{1} = (2n-k-6)\mathbf{1}$. It follows that $q_1(G)$ is bounded above by the Perron value of the 2×2 matrix

$$M = \begin{bmatrix} n-2+k & n-k \\ k & 2n-k-6 \end{bmatrix}.$$

A computation shows that the Perron value of M is given by $\frac{1}{2}(3n-8+\sqrt{n^2-8n+16k+16})$. Since $n \geq 7$ and $k \leq 2$, we find that $\frac{1}{2}(3n-8+\sqrt{n^2-8n+16k+16}) < 2n-4$, and the conclusion follows. ■

Remark 2: For $n = 5$ or $n = 6$ and $k = 1$ vertex of degree $n-1$ and no vertices of degree $n-2$, direct computations show that $q_1 < 2n-4$. However, for $n = 5$ or $n = 6$ and $k = 2$, the graph of the Figure 1 is an example of a graph on n vertices with 2 vertices of degree $n-1$ and no vertices of degree $n-2$ for which $q_1 > 2n-4$.

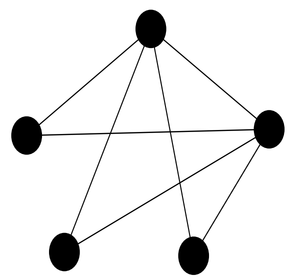

Fig. 1. Graph with 5 vertices, $k = 2$ and $q_1(G) = 6.3722 > 2n - 4$

Lemma 11 *Let G be a graph on n vertices with $k = 1$ or 2 vertices of degree $n-1$, and at least one vertex of degree $n-2$. If $n \geq 7$, then $q_n(G) \geq \frac{2k}{n-2}$.*

PROOF. There is a labelling of the vertices of G such that $Q(G) - T$ is a positive semidefinite matrix, where T is given by

$$T = \left[\begin{array}{c|c|c|c} (n-2)I + J & \mathbf{1} & \mathbf{J} & \mathbf{1} \\ \hline \mathbf{1}^T & n-2 & \mathbf{1}^T & 0 \\ \hline \mathbf{J}^T & \mathbf{1} & (k+1)I & \mathbf{0} \\ \hline \mathbf{1}^T & 0 & \mathbf{0}^T & k \end{array}\right],$$

and where the diagonal blocks are of orders $k, 1, n-k-2$, and 1, respectively.

The eigenvalues of T consist of $n-2$ (with multiplicity $k-1$), $k+1$ (with multiplicity $n-k-3$) and the eigenvalues of the 4×4 matrix

$$U = \begin{bmatrix} n-2+k & 1 & n-k-2 & 1 \\ k & n-2 & n-k-2 & 0 \\ k & 1 & k+1 & 0 \\ k & 0 & 0 & k \end{bmatrix}.$$

Consider $c = \frac{2k}{n-2}$. It suffices to show that the smallest eigenvalue of U is at least c; observing that U is diagonally similar to the symmetric matrix

$$W = \begin{bmatrix} n-2+k & \sqrt{k} & \sqrt{k(n-k-2)} & \sqrt{k} \\ \sqrt{k} & n-2 & \sqrt{n-k-2} & 0 \\ \sqrt{k(n-k-2)} & \sqrt{n-k-2} & k+1 & 0 \\ \sqrt{k} & 0 & 0 & k \end{bmatrix},$$

we find that it is enough to show that $W - cI$ is a positive definite matrix.

We proceed to do so by considering the trailing principal minors of $W - cI$. Evidently $k+1-c > k-c > 0$, while the trailing principal minor of order 3 is $(k-c)((k+1)(n-2) - c(n+k-1) + c^2 - n + k + 2)$. This last is positive if and only if $k(n-3) + \frac{4k^2}{(n-2)^2} > \frac{2k(k+1)}{n-2}$, which clearly holds for $n \geq 5$.

It remains only to check that $\det(W - cI) > 0$. An uninteresting computation shows that $\det(W-cI) = (k-c)[k(k+1)n - 2k(k+1) + 2kn + k^2(n-2) - 5k - 2k^2 - c(n-2)(n-2+k) - c(k+1)(n-2) - 2k(k+1)c + kc + c^2(2n+2k-3) - c^3] - k^2(n-3) - \frac{4k^3}{(n-2)^2} + \frac{2k^2(k+1)}{n-2}$. It follows that $\det(W-cI) > (k-c)[n(2k^2 + 1) - 2k(k+1) - 5k - 2k^2 - 2k^2 - 2k(k+1) - 2k(k+1)c] - k^2(n-3) - \frac{4k^3}{(n-2)^2} > n(2k^3 + k - 2ck^2 - c - k^2) - k((6+c)k(k+1) + 2k^2 + 5k) + 3k^2 - \frac{4k^3}{(n-2)^2}$.

For $k = 1$, that last member is $n(2-3c) - (19+6c) + 3 - \frac{4}{(n-2)^2} = 2n - \frac{6n-12}{n-2} - 16\frac{4}{(n-2)^2}$, which is positive for $n > 12$. For $k = 2$, that last member is $14n - \frac{36n+48}{n-2} + 12 - 108 - \frac{32}{(n-2)^2}$, which again is positive for $n > 12$. Thus, $W - cI$ is positive definite. By direct computation, it turns out that for $k = 1$ or $k = 2$ and $7 \leq n \leq 12$, $\det(W - cI) > 0$, and the conclusion follows. ■

Remark 3: The graph of the Figure 2 is an example of a graph on $n = 6$ vertices with $k = 1$ vertex of degree $n-1$ and at least one vertex of degree $n-2$, for which $q_1 < \frac{2k}{n-2}$.

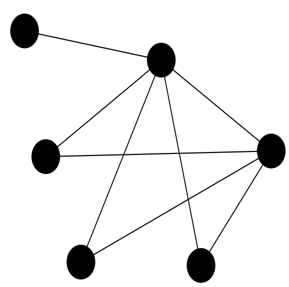

Fig. 2. Graph with 6 vertices, $q_6(G) = 0.48 < \frac{2k}{n-2} = 0.5$

Theorem 12 *Let G be a connected graph on $n \geq 5$ vertices. Then $s_Q(G) < 2n - 4$.*

PROOF. We begin by observing that $s_Q(K_n) = n < 2n-4$ since $n \geq 5$. Henceforth we assume that G is not a complete graph. Suppose first that the maximum degree of G is at most $n-2$. Then the result follows from Lemma 4. Henceforth, we assume that G has $k \geq 1$ vertices of degree $n-1$. If $k \geq 3$, then by Lemma 9 we have $s_Q(G) < 2n-4$ for $n \geq 8$; direct computation for the cases $n = 5, 6, 7$ also yields $s_Q(G) < 2n-4$ by Lemma 8. If $k = 1$ or $k = 2$ and G has no vertices of degree $n-2$, then by Lemma 10, we have $s_Q(G) < 2n-4$

if $n \geq 7$. Finally, if $k = 1$ or $k = 2$ and G has a vertex of degree $n-2$, we find from Lemma 11, $q_n(G) \geq \frac{2k}{n-2}$ for $n \geq 7$. Hence, $s_Q(G) < 2n-4$ for $n \geq 7$, while direct computation for the cases $n = 5, 6$ also yields $s_Q(G) < 2n-4$. ■

Remark 4: It is interesting to note that the conclusion of Theorem 12 fails when $n = 4$. Indeed, direct computations show that of the six connected graphs on four vertices, only the graph P_4 has a Q-spread that is less than $2n-4 = 4$.

Corollary 13 *Let G be a graph on $n \geq 5$ vertices. Then $s_Q(G) \leq 2n-4$. Equality holds if and only if $G = K_{n-1} \cup K_1$.*

PROOF. Suppose first that G is connected. Then the results follows immediately from Lemma 4 and Theorem 12. Suppose now that G is not connected; let C be the connected component of G having the largest number of vertices, and suppose that C has m vertices. We find readily that $q_1(G) \leq 2(m-1) \leq 2n-4$. Hence, we see that $s_Q(G) \leq 2n-4$. Further, if $s_Q(G) = 2n-4$, then we must have that $m = n-1$ and that $q_1(G) = 2n-4$. This last implies that $C = K_{n-1}$, and hence that $G = K_{n-1} \cup K_1$. ■

3 Q-spread of $PC_{n,p,1}$

From now on, we work with graphs of order n obtained from the disjoint union of stars $K_{1,n-p-1}$ and p copies of isolated vertices, pK_1, where $1 \leq p \leq n-2$. Its complement is a special case of the path complete graphs(see [2]), which is denoted as $PC_{n,p,1} = \overline{K_{1,n-p-1} \cup pK_1}$. Several systems for obtaining conjectures in a computer-assisted way have been proposed in the literature. Among them, we employed the AutoGraphix system (AGX) [3]. A survey is available in Caporossi and Hansen [3]. We used AGX to find connected graphs on n vertices with maximum Q-spread. Based on the results of a number of AGX searches, we conjecture that the path complete graph on n vertices has maximum $s_Q(G)$ and it is obtained by adding exactly one edge to the graph $K_{n-1} \cup K_1$. Further, from Corollary 13, the disconnected graph $K_{n-1} \cup K_1$ maximizes the Q-spread over all simple graphs on $n \geq 5$ vertices.

In Theorem 14, we determine the spectrum, and hence the spread, of the graph $PC_{n,p,1}$. Note that in the statement of that theorem, a superscript denotes the multiplicity of the eigenvalue.

Theorem 14 *Let $n \geq 4$ and $G = PC_{n,p,1}$. Then, the spectrum of $PC_{n,p,1}$ is $Spec(Q(PC_{n,p,1})) =$*

$(\frac{2n+p-4\pm\sqrt{4n^2+n(-4p-16)+p^2+16p+16}}{2}, (n-2)^{(p)}, (n-3)^{(n-p-2)})$ *and the spread of* G *is*

$$s_Q(PC_{n,p,1}) = \sqrt{4n^2+n(-4p-16)+p^2+16p+16}.$$

PROOF. We we find that $Q(PC_{n,p,1})$ can be written as

$$Q(PC_{n,p,1}) = \left[\begin{array}{c|c|c} (n-3)I+J & J & \mathbf{0} \\ \hline J & (n-2)I+J & \mathbf{1} \\ \hline \mathbf{0}^T & \mathbf{1}^T & p \end{array}\right],$$

where the diagonal blocks are of orders $n-p-1, p$ and 1, respectively. For each $i = 1, \ldots, n$, let e_i denote the i-th standard unit basis vector. We find that for each $j = 2, \ldots, n-p-1, e_1 - e_j$ is an eigenvector for $Q(PC_{n,p,1})$ corresponding to eigenvalue $n-3$, while for each $j = n-p+1, \ldots, n-1, e_{n-p} - e_j$ is an eigenvector for $Q(PC_{n,p,1})$ corresponding to eigenvalue $n-2$. Consequently, we see that $Q(PC_{n,p,1})$ has $n-3$ as an eigenvalue of multiplicity at least $n-p-2$, and $n-2$ as an eigenvalue of multiplicity at least $p-1$. Further, since $Q(PC_{n,p,1})$ has an orthogonal basis of eigenvectors, it follows that there are remaining eigenvectors of $Q(PC_{n,p,1})$ of the form $\left[\begin{array}{c} \alpha\mathbf{1} \\ \hline \beta\mathbf{1} \\ \hline \gamma \end{array}\right]$. We then deduce that the eigenvalues of the 3×3 matrix $M = \begin{bmatrix} 2n-p-4 & p & 0 \\ n-p-1 & n-2+p & 1 \\ 0 & p & p \end{bmatrix}$ comprise the remaining three eigenvalues of $Q(PC_{n,p,1})$. Direct computation shows that the eigenvalues of M are $\frac{2n+p-4\pm\sqrt{4n^2+n(-4p-16)+p^2+16p+16}}{2}$ and $n-2$.

The expressions for $Spec(Q(PC_{n,p,1}))$ and $s_Q(PC_{n,p,1})$ now follow readily. ■

The following proposition shows that $PC_{n,1,1}$ has maximum Q-spread among all $PC_{n,p,1}$ for $2 \leq p \leq n-2$.

Proposition 15 *For* $n \geq 7$ *and* $2 \leq p \leq n-2$, *we have*

$$s_Q(PC_{n,p+1,1}) < s_Q(PC_{n,p,1}) \leq s_Q(PC_{n,1,1}) = \sqrt{4n^2-20n+33}.$$

PROOF. Observe that the inequality $s_Q(PC_{n,p+1,1}) < s_Q(PC_{n,p,1})$ is equivalent to the inequality $-4n+2p+17 < 0$. Since $p \leq n-2$, we find that

$-4n+2p+17 \le -2n+13 \le -1$, the last inequality following from the hypothesis that $n \ge 7$. Therefore, for $n \ge 7$, we have $s_Q(PC_{n,p+1,1}) < s_Q(PC_{n,p,1})$, as desired. ■

From AutoGraphiX computational tests, we formulate the following conjecture.

Conjecture 16 *For any connected graph G with $n \ge 5$ vertices,*

$$s_Q(G) \le \sqrt{4n^2 - 20n + 33}.$$

The upper bound is attained if and only if $G = PC_{n,1,1}$.

The conjecture above is equivalent to:

Conjecture 17 *There is no connected graph G with $n \ge 5$ vertices such that*

$$\sqrt{4n^2 - 20n + 33} < s_Q(G) < 2n - 4.$$

Observe that $2n - 5 + \frac{2}{n} < \sqrt{4n^2 - 20n + 33}$ for each $n \ge 1$.

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References

[1] Y. Bao, Y. Tan, Y. Fan, The Laplacian spread of unicyclic graph, Applied Mathematics Letters (2009), to appear.

[2] S. Belhaiza, P. Hansen, N. M. M. Abreu and C. S. Oliveira, Variable Neighborhood Sarch for Extremal Graphs XI.: Bounds on Algebraic Connectivity, Graph Theory and Combinatorial Optimization, ed. Springer, (2005), 1–16.

[3] G. Caporossi and P. Hansen, Variable neighborhood search for extremal graphs: the AutographiX system, Discrete Mathematics, **212**, (2000), 29–34.

[4] D. Cvetković, Signless Laplacians and line graphs, Bulletin T. CXXXI de l' Académie serbe des sciences et des arts (2005) Classe des Sciences mathématiques et naturelles Sciences mathématiques, **30**, (2005), 85–92.

[5] D. Cvetković, P. Rowlinson and S. Simić, Signless Laplacian of finite graphs, Linear Algebra and its Applications, **423**, (2007), 155–171.

[6] D. Cvetković, P. Rowlinson and S. Simić, Eigenvalue bounds for the signless Laplacian, Publ. Inst. Math. (Beograd), **81(95)**, (2007), 11–27.

[7] D. A. Gregory, D. Hershkowitz and S. J. Kirkland, The spread of the spectrum of a graph, Linear Algebra and its Applications, **332–334**, (2001), 23–35.

[8] F. Harary, The Maximum Connectivity of a Graph, Proc. Nat. Acad. Sci. U. S., **48**, (1962), 1142–1146.

[9] E. Jiang and X. Zhan, Lower Bounds for the Spread of a Hermitian Matrix, Linear Algebra and its Applications, **256**, (1997), 153–163.

[10] B. Liu and L. Mu-huo, On the spread of the spectrum of a graph, Discrete Mathematics (2008), to appear.

[11] J. Kaarlo Merikoski and R. Kumar, Characterizations and lower bounds for the spread of a normal matrix, Linear Algebra and its Applications, **364**, (2003), 13–31.

[12] L. Soltès, Transmission in graphs: a bound and vertex removing, Math. Slovaca, **41**, **1**, (1991), 11–16.

[13] C. Yan, Properties of spectra of graphs and line graphs, Appli. Math. J. Chinese Univ. Ser.B, **3**, (2002), 371–376.

[14] Y. Zheng Fan, J. Xu, Y. Wang, D. Liang, The Laplacian Spread of a Tree, Discrete Mathematics and Theoretical Computer Science, **10:1**, (2008), 79–86.