Note on the distance spectral gap of graphs

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Abstract

The distance spectral gap of a connected graph is defined as the difference between its first and second distance eigenvalues. In this note, the unique n-vertex trees with minimal and maximal distance spectral gaps, and the unique n-vertex unicyclic graph with minimal distance spectral gap are determined.

Keywords: distance matrix, distance eigenvalue, distance spectral gap, tree, unicyclic graph

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1 Introduction and preliminaries

We consider simple undirected graphs. Let G be a connected graph with vertex set $V(G) = \{v_1, \dots, v_n\}$. For $1 \le i, j \le n$, the distance between vertices v_i and v_j in G, denoted by $d_G(v_i, v_j)$, is the length of a shortest path connecting v_i and v_j in G. The distance matrix of G is the $n \times n$ matrix $D(G) = (d_{ij})$, where $d_{ij} = d_G(v_i, v_j)$. Since $D(G)$ is a symmetric matrix, its eigenvalues are all real numbers. The distance eigenvalues of G are the eigenvalues of $D(G)$, denoted by $\lambda_1(G), \dots, \lambda_n(G)$, arranged in non-increasing order. For $1 \le k \le n$, $\lambda_k(G)$ is called the kth distance eigenvalue of G.

The study of distance eigenvalues dates back to the classical work of Graham and Pollack [6], Edelberg et al. [4] and Graham and Lovász [5] in 1970s. The first distance eigenvalue (also known as the distance spectral radius) has received much attention. Ruzieh and Powers [10] showed that the path P_n is the unique n-vertex connected graph with maximal first distance eigenvalue, while the complete graph K_n is the unique n-vertex

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connected graph with minimal first distance eigenvalue. Moreover, Stevanović and Ilić [11] showed that the star S_n is the unique n-vertex tree with minimal first distance eigenvalue. Recently, the second distance eigenvalue has also received some attention. Xing and Zhou [13] characterized all connected graphs with second distance eigenvalue in $(-\infty, -2+\sqrt{2})$, as well as all trees and unicyclic graphs whose second distance eigenvalues belong to$(-\infty, -\frac{1}{2})$ with exception of a particular type of unicyclic graphs.

It is known that the spectral gap of a graph is defined as the difference between the largest and the second largest eigenvalues of its adjacency matrix [7]. The distance spectral gap of a connected graph G, denoted by $\zeta(G)$, is defined by the difference between its first and second distance eigenvalues, i.e., $\lambda_1(G)-\lambda_2(G)$. Since $D(G)$ is irreducible and nonnegative, by Perron-Frobenius theorem [9, p. 11], $\lambda_1(G)$ is of multiplicity 1, which implies that $\zeta(G) > 0$.

In this note, we investigate the distance spectral gap of trees and unicyclic graphs. We determine the unique n-vertex trees with minimal and maximal distance spectral gaps, and the unique n-vertex unicyclic graph with minimal distance spectral gap, respectively. We also propose a conjecture about the unicyclic graph with maximal distance spectral gap.

Throughout this article, the following notations and lemma are used repeatedly.

For an $n \times n$ matrix M, let $\mu_1(M), \ldots, \mu_n(M)$ be the eigenvalues of M (arranged in non-increasing order if $\mu_1(M), \ldots, \mu_n(M)$ are all real numbers). Let A be an $n \times n$ symmetric matrix, and B an $m \times m$ principal submatrix of A. The interlacing theorem [8, pp. 185–186] states that $\mu_{n-m+i}(A) \le \mu_i(B) \le \mu_i(A)$ for $1 \le i \le m$.

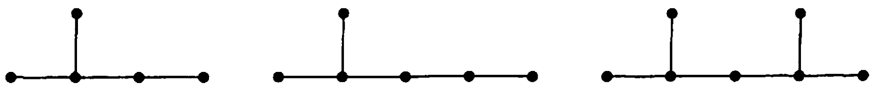
Let G be a nontrivial connected graph, and H a nontrivial induced subgraph of G. If H is connected and $d_H(u,v) = d_G(u,v)$ for all $\{u,v\} \subseteq V(H)$, then write $H \trianglelefteq G$. If $H \trianglelefteq G$, then $D(H)$ is a principal submatrix of $D(G)$, and thus

Lemma 1. *Let G be a nontrivial connected graph, and H a nontrivial induced subgraph of G with $H \trianglelefteq G$. Then $\lambda_2(G) \ge \lambda_2(H)$.*

Let I_n be the $n \times n$ identity matrix, and $J_{m\times n}$ the $m \times n$ all-one matrix. For convenience, let $J_n = J_{n\times n}$ and $\mathbf{1}_n = J_{n\times 1}$.

2 The distance spectral gap of trees

Lemma 2. *[13] Let T be a nontrivial tree. Then $\lambda_2(T) \in (-\infty, -\frac{1}{2})$ if and only if $T \cong S_n$ or P_n for some $n \ge 2$, or one of the three graphs T_1, T_2, T_3 shown in Figure 1.*



T_1 T_2 T_3

Figure 1: Graphs T_1, T_2 and T_3 in Lemma 2.

Lemma 3. *[3] For $n \geq 2$, $\lambda_{1,2}(S_n) = n - 2 \pm \sqrt{n^2 - 3n + 3}$.*

For $n \geq 4$, let D_n be the n-vertex tree obtained by attaching a pendant vertex to a pendant vertex of S_{n-1}.

Lemma 4. *[12] Let T be an n-vertex tree different from S_n, where $n \geq 4$. Then $\lambda_1(T) \geq \lambda_1(D_n)$ with equality if and only if $T \cong D_n$.*

Lemma 5. *For $n \geq 5$, $\lambda_1(D_n) > 2\sqrt{n^2 - 3n + 3}$.*

Proof. If $n = 5, 6, 7, 8$, then by direct check, the result follows easily. Suppose that $n \geq 9$.

Let $v_1v_2v_3v_4$ be a diametrical path of D_n, where v_2 is of degree 2 in D_n, and let $v_5, \ldots, v_n$ be the pendant neighbors of v_3 different from v_4 in D_n. Then

$$D(D_n) + 2I_n = \begin{pmatrix} 2 & 1 & 2 & 3\mathbf{1}_{n-3}^{\mathrm{T}} \\ 1 & 2 & 1 & 2\mathbf{1}_{n-3}^{\mathrm{T}} \\ 2 & 1 & 2 & \mathbf{1}_{n-3}^{\mathrm{T}} \\ 3\mathbf{1}_{n-3} & 2\mathbf{1}_{n-3} & \mathbf{1}_{n-3} & 2J_{n-3} \end{pmatrix}.$$

Since the eigenvalues of $D(D_n)$ are $\lambda_1(D_n), \ldots, \lambda_n(D_n)$, the eigenvalues of $D(D_n) + 2I_n$ are given by $\lambda_1(D_n) + 2, \ldots, \lambda_n(D_n) + 2$, arranged in nonincreasing order. It is easily seen that $D(D_n) + 2I_n$ is of rank 4, which implies that 0 is an eigenvalue of $D(D_n) + 2I_n$ with multiplicity $n - 4$. It is also easily seen that the above partition for $D(D_n) + 2I_n$ is equitable, and thus the eigenvalues of its quotient matrix B are also the eigenvalues of $D(D_n) + 2I_n$ [2, pp. 24–25], where

$$B = \begin{pmatrix} 2 & 1 & 2 & 3(n-3) \\ 1 & 2 & 1 & 2(n-3) \\ 2 & 1 & 2 & n-3 \\ 3 & 2 & 1 & 2(n-3) \end{pmatrix}.$$

Let $f(\lambda)$ be the characteristic polynomial of B. Then we have

$$f(\lambda) = \lambda^4 - 2n\lambda^3 - 2(n-6)\lambda^2 + 16(n-3)\lambda - 12n + 36.$$

Obviously, $\lambda_1(D_n)+2=\mu_1(B)$ is the largest root of $f(\lambda)=0$. By direct calculation, we have $f(2n)=-4(n-1)(2n^2-18n+9)<0$, which, together with the fact that $f(\lambda)\ge 0$ for $\lambda\ge\mu_1(B)=\lambda_1(D_n)+2$, implies that $\lambda_1(D_n)+2>2n$, i.e., $\lambda_1(D_n)>2n-2$. Since $2\sqrt{n^2-3n+3}<2\sqrt{n^2-2n+2}=2n-2$, the result follows. □

Theorem 1. *Let T be a tree on $n\ge 2$ vertices. Then*

$$\varsigma(S_n)\le\varsigma(T)\le\varsigma(P_n)$$

with left equality if and only if $T\cong S_n$, and right equality if and only if $T\cong P_n$.

Proof. The cases $n=2,3$ are trivial. If $n=4$, then $T\cong S_4$ or P_4, and by direct check, $\varsigma(S_4)=2\sqrt{7}<\varsigma(P_4)=4+\sqrt{10}-\sqrt{2}$, which implies the desired result.

If $T\cong T_1$, T_2 or T_3, then by direct calculation, we have $\varsigma\left(S_{|V(T)|}\right)<\varsigma(T)<\varsigma\left(P_{|V(T)|}\right)$.

Suppose in the following that $n\ge 5$, and that $T\ncong S_n$, P_n, T_1, T_2 and T_3. It is sufficient to show that $\varsigma(S_n)<\varsigma(T)<\varsigma(P_n)$.

It is known that $\lambda_1(T)<\lambda_1(P_n)$ [10]. By Lemma 2, we have $\lambda_2(T)>\lambda_2(P_n)$. Thus, $\varsigma(T)=\lambda_1(T)-\lambda_2(T)<\lambda_1(P_n)-\lambda_2(P_n)=\varsigma(P_n)$.

It is also known that $\lambda_2(T)\le 0$ [6]. By Lemma 3, $\lambda_1(S_n)-\lambda_2(S_n)=2\sqrt{n^2-3n+3}$. Then

$$\begin{aligned}\varsigma(T)-\varsigma(S_n) &= \lambda_1(T)-\lambda_2(T)-(\lambda_1(S_n)-\lambda_2(S_n))\\ &\ge \lambda_1(T)-2\sqrt{n^2-3n+3}.\end{aligned}$$

By Lemmas 4 and 5, $\lambda_1(T)\ge\lambda_1(D_n)>2\sqrt{n^2-3n+3}$. Thus $\varsigma(T)>\varsigma(S_n)$. □

3 The distance spectral gap of unicyclic graphs

For an n-vertex connected graph G, let $\sigma(G)=\frac{1}{2}\mathbf{1}_n^{\top}D(G)\mathbf{1}_n$. Obviously, $\sigma(G)$ is just the sum of distances between all unordered pairs of vertices in G, which is known as the transmission (or the Wiener index) of G.

For $n\ge 3$, let S_n^+ be the n-vertex unicyclic graph obtained by adding an edge to the star S_n.

Lemma 6. *[14] Let G be a unicyclic graph on $n\ge 6$ vertices different from S_n^+. Then $\sigma(G)\ge n^2-n-4>\sigma(S_n^+)$.*

Lemma 7. *For $n\ge 9$, we have $\lambda_1(S_n^+)<2n-1-\sqrt{3}-\frac{8}{n}$.*

Proof. Label by $v_1, \dots, v_n$ the vertices of S_n^+, where v_1 is the vertex of maximal degree, v_2 and v_3 are the vertices of degree 2, and $v_4, \dots, v_n$ are the pendant vertices. Then

$$D(S_n^+) + 2I_n = \begin{pmatrix} 2 & 1 & 1 & \mathbf{1}_{n-3}^{\mathsf{T}} \\ 1 & 2 & 1 & 2\mathbf{1}_{n-3}^{\mathsf{T}} \\ 1 & 1 & 2 & 2\mathbf{1}_{n-3}^{\mathsf{T}} \\ \mathbf{1}_{n-3} & 2\mathbf{1}_{n-3} & 2\mathbf{1}_{n-3} & 2J_{n-3} \end{pmatrix},$$

whose eigenvalues are given by $\lambda_1(S_n^+) + 2, \dots, \lambda_n(S_n^+) + 2$. By similar analysis as in the proof of Lemma 5, the eigenvalues of $D(S_n^+) + 2I_n$ consist of 0 with multiplicity $n - 4$, and $\mu_1(B), \mu_2(B), \mu_3(B)$ and $\mu_4(B)$, where

$$B = \begin{pmatrix} 2 & 1 & 1 & n-3 \\ 1 & 2 & 1 & 2(n-3) \\ 1 & 1 & 2 & 2(n-3) \\ 1 & 2 & 2 & 2(n-3) \end{pmatrix}.$$

By direct calculation, the characteristic polynomial of B is $\det(\lambda I_4 - B) = (\lambda - 1)f(\lambda)$, where $f(\lambda) = \lambda^3 - (2n-1)\lambda^2 + (n+1)\lambda + 3n - 9$. Thus, the characteristic polynomial of $D(S_n^+) + 2I_n$ is equal to $\lambda^{n-4}(\lambda - 1)f(\lambda)$. Since S_n^+ is of diameter 2, we have $P_3 \trianglelefteq S_n^+$, and then by Lemma 1, $\lambda_1(S_n^+) + 2 \geq \lambda_2(S_n^+) + 2 \geq \lambda_2(P_3) + 2 = 3 - \sqrt{3} > 1$, implying that $\lambda_1(S_n^+) + 2 = \mu_1(B)$ is the largest root of the equation $f(\lambda) = 0$. By direct calculation, we have

$$\begin{aligned} & n^3 f\left(2n + 1 - \sqrt{3} - \frac{8}{n}\right) \\ = \ & (10 - 4\sqrt{3})n^5 - (13\sqrt{3} + 6)n^4 + (55\sqrt{3} - 98)n^3 + (64\sqrt{3} + 136)n^2 \\ & +(256 - 192\sqrt{3})n - 512 \\ = \ & (10 - 4\sqrt{3})(n-9)^5 + (444 - 193\sqrt{3})(n-9)^4 \\ & +(7786 - 3653\sqrt{3})(n-9)^3 + (67474 - 33929\sqrt{3})(n-9)^2 \\ & +(289444 - 154803\sqrt{3})(n-9) + 492490 - 277938\sqrt{3} \\ > \ & 0, \end{aligned}$$

i.e., $f\left(2n + 1 - \sqrt{3} - \frac{8}{n}\right) > 0$, which, together with the facts that $f(2) = -(3n-5) < 0$ and $f(1) = 2n - 6 > 0$, implies that $\mu_1(B) = \lambda_1(S_n^+) + 2 \in \left(2, 2n + 1 - \sqrt{3} - \frac{8}{n}\right)$, i.e., $\lambda_1(S_n^+) \in \left(0, 2n - 1 - \sqrt{3} - \frac{8}{n}\right)$. □

Theorem 2. *Let G be a unicyclic graph on $n \geq 3$ vertices. Then*

$$\varsigma(G) \geq \varsigma(S_n^+)$$

with equality if and only if $G \cong S_n^+$.

Proof. The case $n = 3$ is trivial. Let G be an n-vertex unicyclic graph different from S_n^+, where $n \geq 4$. It is sufficient to show that $\varsigma(G) > \varsigma(S_n^+)$.

It is known that $\lambda_2(G) \leq 0$ [1]. By Rayleigh-Ritz theorem [8, p. 176] and Lemma 6, we have

$$\lambda_1(G) = \mu_1(D(G)) \geq \frac{\mathbf{1}_n^\top D(G)\mathbf{1}_n}{\mathbf{1}_n^\top \mathbf{1}_n} = \frac{2\sigma(G)}{n} \geq \frac{2(n^2-n-4)}{n} = 2n-2-\frac{8}{n},$$

and thus

$$\begin{aligned} \varsigma(G) - \varsigma(S_n^+) &= \lambda_1(G) - \lambda_2(G) - (\lambda_1(S_n^+) - \lambda_2(S_n^+)) \\ &\geq 2n-2-\frac{8}{n} - \lambda_1(S_n^+) + \lambda_2(S_n^+). \end{aligned}$$

For $n = 4,5,6,7,8$, by direct check, we have $2n-2-\frac{8}{n}-\lambda_1(S_n^+)+\lambda_2(S_n^+) > 0$, which implies the desired result. Suppose that $n \geq 9$. Since S_n^+ is of diameter 2, we have by Lemma 1 that $\lambda_2(S_n^+) \geq \lambda_2(P_3) = 1-\sqrt{3}$, which, together with Lemma 7, implies that

$$2n-2-\frac{8}{n} - \lambda_1(S_n^+) + \lambda_2(S_n^+) \geq 2n-1-\sqrt{3}-\frac{8}{n} - \lambda_1(S_n^+) > 0.$$

Thus the result follows. □

Let $P_n = v_1 \ldots v_n$. Let P_n^+ be the n-vertex unicyclic graph obtained from P_n by adding an edge between v_1 and v_3. Yu et al. [15] showed that P_n^+ is the unique graph with maximal first distance eigenvalue among n-vertex unicyclic graphs. Now we conjecture that for a unicyclic graph G on $n \geq 3$ vertices,

$$\varsigma(G) \leq \varsigma(P_n^+)$$

with equality if and only if $G \cong P_n^+$.

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