



On Pareto eigenvalue of distance matrix of a graph

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Abstract In this article, we study Pareto eigenvalues of distance matrix of connected graphs and show that the non zero entries of every distance Pareto eigenvector of a tree forms a strictly convex function on the forest generated by the vertices corresponding to the non zero entries of the vector. Besides we find the minimum number of possible distance Pareto eigenvalue of a connected graph and establish lower bounds for n largest distance Pareto eigenvalues of a connected graph of order n . Finally, we discuss some bounds for the second largest distance Pareto eigenvalue and find graphs with optimal second largest distance Pareto eigenvalue.

Keywords Pareto eigenvalue · Distance matrix · Spectral radius

Mathematics Subject Classification 05C50 · 05C12

1 Introduction and terminology

All graphs considered here are finite, undirected, connected and simple. Let G be a graph on vertices $1, 2, \dots, n$. At times, we use $V(G)$ and $E(G)$ to denote the set of vertices and the set of edges of G , respectively. For $i, j \in V(G)$, the *distance* between i and j , denoted by $d_G(i, j)$ or simply d_{ij} , is the length of a shortest path from i to j in G . The *distance matrix* of G , denoted by $\mathcal{D}(G)$ is the $n \times n$ matrix with (i, j) -th entry d_{ij} . For a column vector $x = (x_1, \dots, x_n)^T \in \mathbb{R}^n$ we have

$$x^T \mathcal{D}(G) x = \sum_{1 \leq i < j \leq n} d_{ij} x_i x_j.$$

If vertices i and j are adjacent, we write $i \sim j$. Edges e_1, e_2 in a graph G are said to be incident if they have a common vertex. If $V_1 \subseteq V(G)$ and $E_1 \subseteq E(G)$, then by $G - V_1$ and $G - E_1$ we mean the graphs obtained from G by deleting the vertices in V_1 and the edges E_1 respectively. In particular case when $V_1 = \{u\}$ or $E_1 = \{e\}$, we simply write $G - V_1$ by $G - u$ and $G - E_1$ by $G - e$ respectively. $K_n - e$ is the graph obtained from K_n by removing any one edge of it. Degree of a vertex v in a graph G will be denoted by d_v . By a pendent vertex of a graph we mean a vertex of degree 1. For a connected graph G a block B is said to be a pendent block if exactly one vertex of B is a cut vertex of G . A *quasipendent vertex* is a vertex which is adjacent to a pendent vertex. The *transmission*, denoted by $Tr(v)$ of a vertex v is the sum of the distances

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from v to all other vertices in G . The *Wiener index*, denoted by W of a connected graph G is defined as $W = \frac{1}{2} \sum_{v \in V(G)} \text{Tr}(v)$. By P_n , K_n and C_n we mean the usual path graph, complete graph and cycle graph with n vertices respectively. The *diameter* of a connected graph G denoted by $\text{diam}(G)$ is the maximum distance between any two vertices in G , i.e. $\text{diam}(G)$ is the largest entry of $\mathcal{D}(G)$. A *clique* of a graph is a maximal complete subgraph and *clique number* of a graph is the order of a maximal clique. We denote *clique number* of a graph G by $\omega(G)$. For $1 \leq p \leq \omega$ by K_{ω}^p we denote a graph obtained by joining one vertex to p vertices of K_{ω} . By S_n we mean the usual star graph $K_{1,n-1}$ and by S_n^+ we represent the graph so that $S_n^+ - e = S_n$. The graph obtained from G and H by identifying $u \in G$ and $v \in H$ is denoted by $G_u * H_v$ or simply by $G * H$ when there is no confusion of the vertices. We write $H_{u,v}$ to denote a graph of order n with $u, v \in V(H_{u,v})$ so that $d_u = n - 1$ and each vertex in $V(H) - \{u, v\}$ has same vertex degree and same transmission.

By *spectral radius* of a symmetric matrix M , we mean its largest eigenvalue and denote it by $\rho(M)$. Note that for a connected graph G , $\mathcal{D}(G)$ is irreducible nonnegative matrix. Thus by the Perron-Frobenius theorem, $\rho(\mathcal{D})$ is simple, and there is a positive eigenvector of $\mathcal{D}(G)$ corresponding to $\rho(\mathcal{D})$. Such eigenvectors corresponding to $\rho(\mathcal{D})$ is called *Perron vector* of $\mathcal{D}(G)$. By an eigenvector we mean a unit eigenvector and by $\mathbb{M}_n$, we denote the class of all real matrices of order n . We use the notation $A \geq 0$ to indicate that each entry of the matrix A is nonnegative. Furthermore, in places we write $A \geq B$ to mean $A - B \geq 0$.

Definition 1.1 A real number λ is said to be a Pareto eigenvalue of $A \in \mathbb{M}_n$ if there exists a nonzero vector $\mathbf{x}(\geq 0) \in \mathbb{R}^n$ such that

$$A\mathbf{x} \geq \lambda\mathbf{x} \quad \text{and} \quad \lambda = \frac{\mathbf{x}^T A \mathbf{x}}{\mathbf{x}^T \mathbf{x}},$$

also we call $\mathbf{x}$ to be a Pareto eigenvector of A associated with Pareto eigenvalue λ .

Pareto eigenvalues are also known as complementarity eigenvalues. Fernandes *et al.* [3] and Seeger [7] studied the Pareto eigenvalues of adjacency matrix of a graph.

We now outline the contents of this article. In Section 2, we introduce distance Pareto eigenvalue (eigenvector) of a connected graph and show that non zero entries of every distance Pareto eigenvector of a tree forms a strictly convex function on the forest generated by vertices corresponding to the non zero entries of the vector. We also find the complete distance Pareto spectrum for some special class of graphs like complete graph, star graph etc. Partial distance Pareto spectrum of graphs with given diameter or given clique number are also supplied. Besides we find the minimum number of possible distance Pareto eigenvalue of a connected graph and establish lower bounds for n largest distance Pareto eigenvalues of a connected graph of order n , equality conditions have also been established. In Section 3, we discuss the second largest distance Pareto eigenvalue of a connected graph, specially we give some bounds for it and find graphs with optimal second largest distance Pareto eigenvalue.

2 Distance Pareto eigenvalue of a connected graph

Definition 2.1 Distance Pareto eigenvalue of a connected graph G is a Pareto eigenvalue of the distance matrix of G .

Although significant works have been done for Pareto eigenvalues of the adjacency matrix of graph, but the study of distance Pareto eigenvalues has not been found in the literature. Therefore it needs to be explored and we can expect some remarkable results in this direction. Multiplicity of Pareto eigenvalue of a matrix is not considered. We denote the k^{th} largest and k^{th} smallest distance Pareto eigenvalue of a connected graph G by $\rho_k(G)$ and $\mu_k(G)$ respectively. We simply write them by ρ_k and μ_k when the graph under consideration is understood from the context. Besides we use $\Pi(G)$ to denote the set of all distance Pareto eigenvalues of a connected graph G .

We write $[n] = \{1, 2, \dots, n\}$ and for an $n \times n$ matrix A and $S \subset [n]$, we reserve the symbol $A(S)$ for the principal submatrix of A obtained by deleting rows and columns of A corresponding to S . In particular if $\mathcal{D}(G)$ is the distance matrix of a graph G then by $\mathcal{D}(i)$ we will denote the principal submatrix of $\mathcal{D}$ obtained by deleting row and column corresponding to vertex i of G . By $\mathbb{1}$ we denote the column vector of all ones and by $\mathbb{J}$ the matrix of all ones of appropriate size. We now recall some known results which will be used.



Lemma 2.2 [Weyl's Inequalities] [4] Let $\lambda_i(M)$ denote the i -th largest eigenvalue of a real symmetric matrix M . If A and B are two real symmetric matrices of order n , then

$$\lambda_1(A) + \lambda_i(B) \geq \lambda_i(A+B) \geq \lambda_n(A) + \lambda_i(B) \text{ for } i = 1, 2, \dots, n.$$

Lemma 2.3 [5] If A is an irreducible matrix and $A \geq B \geq 0, A \neq B$, then $\rho(A) > \rho(B)$.

Lemma 2.4 [Cauchy's Inequalities] [4] Let $A = \begin{pmatrix} B & y \\ y^T & a \end{pmatrix} \in \mathbb{M}_{n+1}$ with $y \in \mathbb{C}^n, a \in \mathbb{R}$ and $B \in \mathbb{M}_n$ be symmetric. Then

$$\lambda_1(A) \leq \lambda_1(B) \leq \lambda_2(A) \leq \dots \leq \lambda_n(A) \leq \lambda_n(B) \leq \lambda_{n+1}(A),$$

where $\lambda_i(N)$ is the i^{th} smallest eigenvalue of N . Also $\lambda_i(A) = \lambda_i(B)$ if and only if there is a non zero vector $z \in \mathbb{C}^n$ such that $Bz = \lambda_i(B)z, y^T z = 0$ and $Bz = \lambda_i(A)z$.

Lemma 2.5 [4] Let $A, B \in \mathbb{M}_n$ be nonnegative where A is irreducible and B is non zero, then $\rho(A+B) > \rho(A)$.

Lemma 2.6 [4] If A is a symmetric $n \times n$ matrix with λ_1 as the largest eigenvalue then for any normalized vector $\mathbf{x} \in \mathbb{R}^n (\mathbf{x} \neq 0)$,

$$\mathbf{x}^T A \mathbf{x} \leq \lambda_1.$$

The equality holds if and only if $\mathbf{x}$ is an eigenvector of A corresponding to the eigenvalue λ_1 .

Putting $\mathbf{x} = \frac{1}{\sqrt{n}} \mathbb{1}$ in Lemma 2.6 we get the following result as a Corollary.

Corollary 2.7 If A is a symmetric $n \times n$ matrix, then

$$\rho(A) \geq \bar{R}, \quad (2.1)$$

where $\bar{R}$ is the average row sum of the matrix A . The equality in 2.1 holds if and only if all the row sums of A are equal.

Theorem 2.8 [6] The scalar $\lambda \in \mathbb{R}$ is a Pareto eigenvalue of $A \in \mathbb{M}_n$ if and only if there exists a nonempty set $J \subset \{1, 2, \dots, n\}$ and a vector $\xi \in \mathbb{R}^{|J|}$ such that

$$\begin{aligned} A^J \xi &= \lambda \xi, \text{ where } A^J = [a_{ij}]_{i,j \in J} \\ \xi_j &> 0 \quad \text{for all } j \in J, \\ \sum_{j \in J} a_{ij} \xi_j &\geq 0 \quad \text{for all } i \notin J. \end{aligned}$$

Furthermore, a Pareto eigenvector $\mathbf{x}$ associated to λ is constructed by setting

$$\mathbf{x}_j = \begin{cases} \xi_j & \text{if } j \in J, \\ 0 & \text{otherwise.} \end{cases}$$

From Theorem 2.8, we get the following result similar to that of [7, Theorem 1].

Theorem 2.9 The distance Pareto eigenvalues of a connected graph G are given by $\Pi(G) = \{\rho(A) : A \in M\}$, where M is the class of all principal submatrices of $\mathcal{D}(G)$.

From Theorem 2.9, for any connected graph G we see that every Pareto eigenvalue of any principal submatrix of $\mathcal{D}(G)$ is the distance Pareto eigenvalue of G . Therefore as a consequence we get that if G is a connected graph and H is a block of G , then every distance Pareto eigenvalue of H is also a distance Pareto eigenvalue of G . Also if G is a connected graph and H is a subgraph of G obtained by removing one or more pendent blocks of G , then $\lambda \in \Pi(H)$ implies $\lambda \in \Pi(G)$. Again if ω is the clique number of the graph G , then $\mathbb{J}_\omega - I_\omega$ is a principal submatrix of $\mathcal{D}(G)$ and Pareto eigenvalues of $\mathbb{J}_\omega - I_\omega$ are $0, 1, \dots, \omega - 2$ and $\omega - 1$. Therefore $0, 1, \dots, \omega - 1$ are distance Pareto eigenvalues of G . Similarly if there are p vertices in a graph G which are at a distance k from each other, then $k(\mathbb{J}_p - I_p)$ is a principal submatrix of $\mathcal{D}(G)$ and therefore Pareto eigenvalues of $k(\mathbb{J}_p - I_p)$ i.e. $0, k, \dots, k(p-2)$ and $k(p-1)$ are distance Pareto



eigenvalues of G . Besides from Theorem 2.9, we get the following lemma which states that for a connected graph the distance spectral radius and the largest distance Pareto eigenvalue coincide.

Lemma 2.10 *The largest distance Pareto eigenvalue of a connected graph is the distance spectral radius of the graph.*

Definition 2.11 [2] Let T be a tree with $V(T) = \{1, \dots, n\}$, $n \geq 3$, and let $f : V(T) \rightarrow [0, \infty)$. Then f is said to be *convex* if for any distinct $i, j, k \in V(T)$ with $i \sim j, j \sim k$ we have $2f(j) \leq f(i) + f(k)$ and *strictly convex* if $2f(j) < f(i) + f(k)$. Also f is said to be *quasiconvex* if for any distinct $i, j, k \in V(T)$ with $i \sim j, j \sim k$ we have $f(j) \leq \max\{f(i), f(k)\}$ and *strictly quasiconvex* if $f(j) < \max\{f(i), f(k)\}$. A function defined on the vertices of a forest F is said to be convex, strict convex, quasiconvex or strictly quasiconvex if it is so in any subtree of F .

Lemma 2.12 [2] *Let T be a tree with $V(T) = \{1, \dots, n\}$ and let $f : V(T) \rightarrow [0, \infty)$ be either strictly convex or strictly quasiconvex. Then f attains its minimum, either at a unique vertex, or at two adjacent vertices. Furthermore,*

- (i) if f attains its minimum at the unique vertex i , then for any path $i = i_1 - i_2 - \dots - i_k$, starting at i , $f(i_1) < f(i_2) < \dots < f(i_k)$.
- (ii) if f attains its minimum at the two adjacent vertices i and j , then f is strictly increasing along any path starting at i , and not containing j , or starting at j , and not containing i .

Lemma 2.13 [2] *Let $\mathcal{D}$ be the distance matrix of a tree T and let $f : [0, \infty) \rightarrow [0, \infty)$ be a strictly increasing convex function. Then the Perron vector of $f(\mathcal{D})$ is strictly convex on T .*

Theorem 2.14 *If $\mathbf{x}$ is a distance Pareto eigenvector of a tree T and $V_x = \{v \in T : \mathbf{x}_v > 0\}$ then the non zero components of $\mathbf{x}$ form a strictly convex function on the subgraph of T generated by V_x .*

Proof If $\mathbf{x}$ is a distance Pareto eigenvector of tree T with corresponding distance Pareto eigenvalue λ then from Theorem 2.9 and Theorem 2.8, λ is a spectral radius for some principal submatrix M of $\mathcal{D}(T)$ and $x_v > 0$ if and only if v^{th} row(column) of $\mathcal{D}(T)$ is in M . If $\lambda = 0$, then cardinality of V_x is 1 and therefore the result is trivially true. So we assume $\lambda \neq 0$. Now if the subgraph of T generated by V_x is again a tree, then the result follows from Lemma 2.13.

Otherwise, we consider a subtree T' of the subgraph (forest) of T generated by V_x . Let u, v, w be vertices of T' such that $u \sim v \sim w$. Let $e_1 = \{u, v\}$, $e_2 = \{v, w\}$ be edges of T' . Let T_u, T_v and T_w be the components of $T - \{e_1, e_2\}$, containing u, v and w , respectively. From eigenequations of M , we have

$$\begin{aligned} \lambda x_u &= \sum_{y \in T_1 \cap V_x} d_{uy} x_y + \sum_{y \in T_2 \cap V_x} (d_{vy} + 1) x_y \\ &\quad + \sum_{y \in T_3 \cap V_x} g(d_{wy} + 2) x_y \end{aligned} \quad (2.2)$$

$$\begin{aligned} \lambda x_v &= \sum_{y \in T_1 \cap V_x} (d_{uy} + 1) x_y + \sum_{y \in T_2 \cap V_x} d_{vy} x_y \\ &\quad + \sum_{y \in T_3 \cap V_x} (d_{wy} + 1) x_y \end{aligned} \quad (2.3)$$

$$\begin{aligned} \lambda x_w &= \sum_{y \in T_1 \cap V_x} (d_{uy} + 2) x_y + \sum_{y \in T_2 \cap V_x} (d_{vy} + 1) x_y \\ &\quad + \sum_{y \in T_3 \cap V_x} d_{wy} x_y. \end{aligned} \quad (2.4)$$

It follows from (2.2)-(2.4) that

$$\begin{aligned} \lambda(x_u + x_w - 2x_v) &= \sum_{y \in T_2 \cap V_x} 2x_y \\ &\geq 2x_v \\ &> 0 \quad \text{as } x_v > 0 \end{aligned}$$

Thus $x_u + x_w > 2x_v$ as $\lambda > 0$.



As T' is an arbitrary subtree of the subgraph of T generated by V_x , hence the result follows. $\square$

Theorem 2.15 For a connected graph of diameter d , the integers $0, 1, \dots, d$ are always its distance Pareto eigenvalues.

Proof If G is a graph with diameter d , then $\mathcal{D}(P_d)$ is a principal submatrix of $\mathcal{D}(G)$ and therefore by Theorem 2.9 every $\lambda \in \Pi(P_d)$ implies $\lambda \in \Pi(G)$. Let

$$A_k = \begin{pmatrix} 0 & k \\ k & 0 \end{pmatrix}.$$

Then for $1 \leq k \leq d$, A_k is a principal submatrix of $\mathcal{D}(P_d)$ and $\rho(A_k) = k$. Therefore $k \in \Pi(P_d)$ for $1 \leq k \leq d$. Besides 0 being a diagonal element of $\mathcal{D}(P_d)$ is in $\Pi(P_d)$. Hence the result follows. $\square$

As for a complete graph the distance matrix and the adjacency matrix coincide, therefore from [7] we have the following.

Lemma 2.16 [7] For any positive integer n , $\Pi(K_n) = \{0, 1, \dots, n-1\}$.

Definition 2.17 If A and B are two nonnegative matrices then we say that A dominates B if either of the following two cases hold

1. A and B are of same size and up to permutation similarity $A \geq B$, $A \neq B$.
2. A is permutation similar to $\begin{pmatrix} B & C \\ D & E \end{pmatrix}$ and at least one of C, D and E is a nonzero matrix.

From Lemma 2.3, Lemma 2.4 and Lemma 2.5 we get the following.

Lemma 2.18 If A and B are two symmetric nonnegative irreducible matrices, then A dominates B implies $\rho(A) > \rho(B)$.

Lemma 2.19 [1] Distance spectral radius of the star S_n is

$$n-2 + \sqrt{(n-2)^2 + n-1}$$

Theorem 2.20 There are exactly $2(n-1)$ distance Pareto eigenvalues of S_n and they are

$$\mu_{2k-1} = 2(k-1), \mu_{2k} = k-1 + \sqrt{k^2 - k + 1} \text{ where } k = 1, \dots, n-1.$$

Proof Up to permutation similarity there are exactly two distinct principal submatrices of $\mathcal{D}(S_n)$ of order $k = 2, \dots, n-1$ and they are $\mathcal{D}(S_k)$ and $2(\mathbb{J}_k - I_k)$. Clearly the later always dominates the former one.

Besides $\rho(2(\mathbb{J}_k - I_k)) = 2(k-1)$ and from Lemma 2.19, we have $\rho(\mathcal{D}(S_k)) = k-2 + \sqrt{(k-2)^2 + k-1}$.

By routine calculation it can be easily shown that

$$\begin{aligned} \rho(\mathcal{D}(S_{k+1})) &> \rho(2(\mathbb{J}_k - I_k)) \\ &> \rho(\mathcal{D}(S_k)) \text{ for } k = 2, \dots, n-1 \end{aligned} \quad (2.5)$$

As 0 is always a distance Pareto eigenvalue of a connected graph and $\rho(\mathcal{D}(S_n))$ is the largest distance Pareto eigenvalue of S_n , using (2.5) we get all the distance Pareto eigenvalues of S_n as follows

$$\mu_{2k-1} = 2(k-1), \mu_{2k} = \rho(\mathcal{D}(S_{k+1})) \text{ where } k = 1, \dots, n-1.$$

$\square$

Theorem 2.21 If G is a connected graph of order n and diameter d then $|\Pi(G)| \geq n + d - 1$, with equality if and only if $G = P_3$ or K_n .

Proof From Theorem 2.15, we have $0, 1, \dots, d$ as distance Pareto eigenvalues of G . Let $A_2 = \begin{pmatrix} 0 & d \\ d & 0 \end{pmatrix}$.

For $n \leq 2$ there is nothing to prove. If $n \geq 3$ then for $i = 3, \dots, n$ we can have submatrices A_i of $\mathcal{D}(G)$ of order i such that A_i dominates A_{i-1} . Therefore by Lemma 2.18, $\rho(A_i) > \rho(A_{i-1})$. Thus we get $(d+1) + (n-2) = n + d - 1$ distance Pareto eigenvalues of G as follows



$$0 < 1 < \cdots < d < \rho(A_3) < \cdots < \rho(A_n).$$

Hence

$$|\Pi(G)| \geq n + d - 1. \quad (2.6)$$

Now from Lemma 2.16, we have $|\Pi(K_n)| = n$ and by direct calculation $|\Pi(P_3)| = 4$. Therefore for $G = P_3, K_n$ the equality holds in (2.6).

If $G \neq P_3, K_n$ then $n \geq 4$ and $d \geq 2$ and thus $\mathcal{D}(P_3)$ is a principal submatrix of $\mathcal{D}(G)$. For $d \geq 3$ we see that $\rho(\mathcal{D}(P_3)) = 1 + \sqrt{3} < \rho(A_3)$ as minimum row sum of A_3 is at least $d + 1 \geq 4$. Again if $d = 2$ then either

$$P = \begin{pmatrix} 0 & 2 & 2 \\ 2 & 0 & 1 \\ 2 & 1 & 0 \end{pmatrix} \text{ or } Q = 2(\mathbb{J}_3 - I_3) \text{ must be a principal submatrix of } \mathcal{D}(G). \text{ So we can choose } A_3 = P \text{ or}$$

$A_3 = Q$, whichever be the case. Also $1 + \sqrt{3} < \min\{\rho(P), \rho(Q)\}$.

In either situation we get $1 + \sqrt{3} \in \Pi(G)$ in addition to the above listed $n + d - 1$ distance Pareto eigenvalues of G . Thus $|\Pi(G)| \geq n + d$. $\square$

Note: From Theorem 2.21 we see that for any connected graph G with n vertices, $|\Pi(G)| \geq n$ and the equality is achieved if and only if $G = K_n$. But the exact number of distance Pareto eigenvalues of a connected graph of order n is not known. Now for any $n \times n$ matrix there are exactly $2^n - 1$ principal submatrices, so by Theorem 2.9 we can not have more than $2^n - 1$ distance Pareto eigenvalues of any connected graph with n vertices. Also we can see that for any connected graph with $n \geq 2$ vertices, all the principal submatrices of $\mathcal{D}(G)$ are not distinct. Besides we may have some principal submatrices which are distinct but having same spectral radius. Therefore for any connected graph G of order n if there are $s(G)$ distinct principal submatrices of $\mathcal{D}(G)$ then $|\Pi(G)| \leq s(G)$, with equality if and only if all the distinct submatrices of $\mathcal{D}(G)$ have distinct spectral radii. In this regard another question arises that among all connected graphs of given order which graph(s) will have maximum number of distance Pareto eigenvalues. By direct calculation we have seen that among all connected graphs of order $n = 2, 3, 4$ the path graph P_n has the maximum number of distance Pareto eigenvalues. The numbers are respectively 2, 4 and 7. But for graphs of order 5, we see that the path graph P_5 together with graphs G_1 and G_2 of Figure 1 have maximum (here 13) number of distance Pareto eigenvalues. Again for the class of graphs of order 6, the graph G_3 in Figure 1 attains uniquely the maximum (30) number of distance Pareto eigenvalues. Therefore this seems to be an interesting problem to characterize all graphs for which the maximum number of distance Pareto eigenvalues occur among all connected graphs of given order. We here pose a question which perhaps require deep investigation. Can distance Pareto eigenvalues of a connected graph uniquely determine the graph? In addition to that it is worth studying how fast distance Pareto eigenvalues grow when number of vertices increases. We leave these problems for future research scope.

Theorem 2.22 *If G is a graph with n vertices, then*

$$\rho_k(G) \geq n - k \text{ for } k = 1, 2, \dots, n.$$

Equality holds if and only if $G = K_n$.

Proof If $G = K_n$, then using Lemma 2.16 we are done.

If $G \neq K_n$, then for $i = 1, 2, \dots, n - 2$, we can have A_i of order $n - i + 1$ as principal submatrix of $\mathcal{D}(G)$ such that $A_1 = \mathcal{D}(G)$, $A_{n-2} = \mathcal{D}(P_3)$, A_{i+1} is a principal submatrix of A_i for $i = 1, 2, \dots, n - 3$.

Besides A_i dominates $\mathbb{J}_{n-i+1} - I_{n-i+1}$ for $i = 1, 2, \dots, n - 3$.

But

$$\rho(\mathbb{J}_{n-i+1} - I_{n-i+1}) = n - i.$$

$$\text{Therefore } \rho_i(G) > n - i \text{ for } i = 1, 2, \dots, n - 3. \quad (2.7)$$

Now since $A_{n-2} = \mathcal{D}(P_3)$ and $\Pi(P_3) = \{0, 1, 2, 1 + \sqrt{3}\}$, we get

$$\rho_{n-2}(G) \geq 1 + \sqrt{3} > 2, \rho_{n-1}(G) \geq 2 > 1 \text{ and } \rho_n(G) \geq 1 > 0. \quad (2.8)$$

Combining (2.7) and (2.8), we get the result as desired. $\square$



3 Second largest distance Pareto eigenvalue

The largest distance Pareto eigenvalue of a connected graph is nothing but the distance spectral radius of the graph. Also in last few decades distance spectral radius have been extensively studied. In this section we study some bounds for the second largest distance Pareto eigenvalue.

Theorem 3.1 *If G is a connected graph with at least two vertices, then*

$$\rho_2(G) = \max\{\rho(A) : A \in P\},$$

where $P = \{(\mathcal{D}(G))(v) : v \in V(G), d_v > 1\}$

Proof Since $\mathcal{D}(G)$ dominates A for every $A \in P$, we have

$$\rho_2(G) \leq \rho(A) < \rho_1(G) \text{ for every } A \in P.$$

Also for every principal submatrix B of $\mathcal{D}(G)$ of order $n - 2$ or less, there exist $A \in P$ which dominates B and therefore $\rho(B) < \rho(A)$. Thus $\rho_2(G)$ must be equal to the largest $\rho(A)$ for all possible $A \in P$.

Now if u is a pendent vertex in G and v is a quasi-pendent vertex in G adjacent to u , then the principal submatrix of $\mathcal{D}(G)$ obtained by removing row and column corresponding to vertex v dominates the principal submatrix of $\mathcal{D}(G)$ obtained by removing row and column corresponding to vertex u . Therefore in calculating $\rho_2(G)$ we can ignore those principal submatrices of $\mathcal{D}(G)$ which are obtained by removing row and column corresponding to pendent vertex. Hence the result follows. $\square$

Theorem 3.2 *If G is a graph of order n with a vertex of degree $n - 1$, then*

$$n - 2 \leq \rho_2(G) \leq 2(n - 2),$$

the right hand equality holds if and only if $G = S_n$ and the left hand equality holds if and only if $G = K_n$.

Proof From Theorem 2.22, we see that $\rho_2(G) \geq n - 2$ and equality holds if and only if $G = K_n$.

Now suppose $G \neq K_n$. Let $v \in V(G)$ with $d_G(v) = n - 1$. and A be the principal submatrix of $\mathcal{D}(G)$ obtained by deleting row and column of $\mathcal{D}(G)$ corresponding to vertex v . Then Clearly $\rho_2(G) = \rho(A)$, as A dominates any other principal submatrix of $\mathcal{D}(G)$ of order $n - 1$.

From Theorem 2.20, $\rho_2(S_n) = 2(n - 1)$. Now if $G \neq S_n$, then we can find two vertices $u, w (\neq v) \in V(G)$ such that $u \sim w$ in G . Thus $2(\mathbb{J}_{n-1} - I_{n-1})$ dominates A . Therefore $\rho_2(G) = \rho(A) < 2(n - 1)$. $\square$

Theorem 3.3 *If G is a connected graph of order n and diameter 2, then $\rho_2(G) \leq 2(n - 2)$, with equality if and only if $G = S_n$.*

Proof By Theorem 2.20, we have $\rho_2(S_n) = 2(n - 2)$. Now if $G \neq S_n$, then there is at least two non-pendent vertices $u, v \in V(G)$. So there are at least two 1's in each of u -th and v -th rows(columns) of $\mathcal{D}(G)$. Therefore if A is any principal submatrix of $\mathcal{D}(G)$ of order $n - 1$, then clearly $2(\mathbb{J}_{n-1} - I_{n-1})$ dominates A . Thus $2(n - 2) > \rho_2(G)$. $\square$

Theorem 3.4 *If G is a connected graph with n vertices and $\omega(G) \geq n - 1$, then*

$$n - 2 \leq \rho_2(G) \leq \frac{n - 3 + \sqrt{n^2 + 10n - 23}}{2},$$

with equality in the left hand side if and only if $G = K_n$ and equality in the right hand side if and only if $G = K_{n-1}^1$.

Proof From Theorem 2.16, we have $\rho_2(G) \geq n - 2$ with equality if and only if $G = K_n$.

Now as $\omega(G) \geq n - 1$, we can take $H = K_{n-1}$ to be a subgraph of G and $v \in V(G) - V(H)$. Then up to permutation similarity we have

$$\begin{aligned} \mathcal{D}(G) &= \begin{pmatrix} \mathcal{D}(K_{n-1}) & x \\ x^T & 0 \end{pmatrix}, \text{ where } x_u = 1 \text{ if } u \sim v \\ &= 2 \text{ otherwise.} \end{aligned}$$



Since G is connected, there exists $w \in V(H)$ with $w \sim v$. If $B(G)$ is the principal submatrix of $\mathcal{D}(G)$ obtained by deleting row and column corresponding to w then clearly $\rho_2(G) = \rho(B)$. and it can be easily observed that $B(K_{n-1}^p)$ dominates $B(K_{n-1}^{p-1})$ for $p = 2, \dots, n$. Therefore

$$\rho_2(K_{n-1}^1) > \rho_2(K_{n-1}^2) > \dots > \rho_2(K_{n-1}^{n-1}) > \rho_2(K_{n-1}^n)$$

Thus we get $\rho_2(G) \leq \rho(\mathcal{D}(K_{n-1}^1))$, with equality if and only if $G = K_{n-1}^1$.

Now let (ρ, y) be the eigenpair of $B(K_{n-1}^1)$. Then due to symmetry $y_2 = y_3 = \dots = y_{n-1}$.

From eigenequations we have

$$2(n-1)y_2 = \rho y_1 \quad (3.9)$$

$$2y_1 + (n-3)y_2 = \rho y_2 \quad (3.10)$$

From (3.9) and (3.10) we get $\rho^2 - (n-3)\rho - 4(n-2) = 0$. Which gives

$$\rho = \frac{n-3 + \sqrt{n^2 + 10n - 23}}{2}.$$

Hence the result follows. $\square$

Theorem 3.5 For any non-complete connected graph G with n vertices,

$$\rho_2(G) \geq \frac{n-2 + \sqrt{n^2 - 4n + 12}}{2},$$

with equality if and only if $G = K_n - e$.

Proof First we find the expression for $\rho(\mathcal{D}(K_n - e))$. If (ρ, x) is the eigenpair for $\mathcal{D}(K_n - e)$, where $e = \{1, 2\}$. Then due to symmetry we have

$$x_1 = x_2 \text{ and } x_3 = \dots = x_n. \quad (3.11)$$

Also we have

$$\mathcal{D}(K_n - e) = \begin{pmatrix} 0 & 2 & \mathbb{1}_{n-2}^T \\ 2 & 0 & 1 \\ \mathbb{1}_{n-2} & 1 & \mathcal{D}(K_{n-2}) \end{pmatrix} \quad (3.12)$$

Using (3.11) and (3.12) in eigenequations of $\mathcal{D}(K_n - e)$, we get

$$2x_1 + (n-2)x_3 = \rho x_1 \quad (3.13)$$

$$2x_1 + (n-3)x_3 = \rho x_3 \quad (3.14)$$

From (3.13) and (3.14) we have $\rho^2 - (n-1)\rho - 2 = 0$. Thus we get

$$\rho(\mathcal{D}(K_n - e)) = \frac{n-1 + \sqrt{(n-1)^2 + 8}}{2}. \quad (3.15)$$

Clearly $\mathcal{D}(K_{n-1} - e)$ and $\mathbb{J}_{n-1} - I_{n-1}$ are the only two distinct submatrices of $\mathcal{D}(K_n - e)$ of order $n-1$ and the former dominates the later one. Therefore

$$\rho_2(K_n - e) = \rho(\mathcal{D}(K_{n-1} - e)) = \frac{n-2 + \sqrt{n^2 - 4n + 12}}{2} \text{ [using (3.15)]}$$

Now if $G \neq K_n - e$, then any principal submatrix of $\mathcal{D}(G)$ of order $n-1$ dominates $\mathcal{D}(K_{n-1} - e)$ and therefore $\rho_2(G) > \frac{n-2 + \sqrt{n^2 - 4n + 12}}{2}$.

Hence the result follows. $\square$



Corollary 3.6 For any non-complete connected graph G with n vertices,

$$\rho_2(G) \geq n - 2 + \frac{2}{n-1}$$

equality holds if and only if $G = P_3$.

Proof As G is connected and non-complete, therefore $n \geq 3$. Which implies that

$$n^2 - 4n + 12 \geq \left(n - 2 + \frac{4}{n-1}\right)^2.$$

Thus

$$\frac{n - 2 + \sqrt{n^2 - 4n + 12}}{2} \geq n - 2 + \frac{2}{n-1} \quad (3.16)$$

It can be easily shown that equality in (3.16) holds if and only if $n = 3$. Therefore by Theorem 3.5 we get

$$\rho_2(G) \geq n - 2 + \frac{2}{n-1},$$

with equality if and only if $G = K_3 - e = P_3$. $\square$

Theorem 3.7 If G is a connected graph of order n so that minimum transmission occurs at a vertex $v \in G$ and $\mathbf{x}$ is the normalized distance Pareto eigenvector corresponding to ρ_2 , then

$$\rho_2(G) \geq \frac{2[W - \text{Tr}(v)]}{n-1},$$

with equality if and only if $x_u = \frac{1}{\sqrt{n-1}}$ for $u \neq v$.

Proof Let D_v be the submatrix of $\mathcal{D}(G)$ obtained by deleting row and column corresponding to vertex v . Then the average row sum of D_v equals $\frac{2(W - \text{Tr}(v))}{n-1}$. Therefore, using Corollary 2.7, we get

$$\begin{aligned} \rho_2(G) &\geq \rho(D_v) \\ &\geq \frac{2(W - \text{Tr}(v))}{n-1}. \end{aligned}$$

Now equality holds in the above expression if and only if $\rho_2(G) = \rho(D_v)$ and all the row sums of D_v are equal which is the case if and only if $x_v = 0$ and x_u is constant for $u \neq v$. Thus we get the required condition from the facts that $\mathbf{x}$ is normalized and exactly one component of $\mathbf{x}$ is zero. $\square$

Note: The equality in Theorem 3.7 holds for several graphs like complete graph, star graph, wheel graph etc.

Theorem 3.8 For any connected graph G of order n other than K_n and $K_n - e$

$$\rho_2(G) \geq \frac{n - 2 + \sqrt{n^2 - 4n + 20}}{2},$$

with equality if and only if $G = K_n - \{e_1, e_2\}$, where e_1 and e_2 are not incident in K_n .

Proof Let $G_1 = K_n - \{e_1, e_2\}$, where $e_1, e_2 \in E(K_n)$ are not incident and $G_2 = K_n - \{f_1, f_2\}$, where $f_1, f_2 \in E(K_n)$ are incident. Up to permutation similarity there are exactly two distinct principal submatrices of $\mathcal{D}(G_1)$ of order $n-1$ and they are given by

$$\begin{aligned} M &= \begin{pmatrix} 2(\mathbb{J}_2 - I_2) & \mathbb{J}_2 - I_2 & \mathbb{J} - I \\ \mathbb{J}_2 - I_2 & 2(\mathbb{J}_2 - I_2) & \mathbb{J}_2 - I_2 \\ \mathbb{J} - I & \mathbb{J}_2 - I_2 & \mathbb{J} - I \end{pmatrix} \\ \text{and } N &= \begin{pmatrix} 2(\mathbb{J}_2 - I_2) & \mathbb{J} - I \\ \mathbb{J} - I & \mathbb{J} - I \end{pmatrix}. \end{aligned}$$

Clearly M dominates N and therefore $\rho_2(G_1) = \rho(M)$.



If (ρ, x) be the eigenpair of M , then due to symmetry

$$x_1 = x_2 = x_3 = x_4 = a \text{ (say)} \quad (3.17)$$

$$\text{and } x_5 = \cdots = x_n = b \text{ (say)} \quad (3.18)$$

Using (3.17) and (3.18) in eigenequations of M we get

$$2a + 2a + (n-5)b = \rho a \quad (3.19)$$

$$4a + (n-6)b = \rho b \quad (3.20)$$

From (3.19) and (3.20) we get

$$\rho_2(G_1) = \rho(M) = \frac{n-2 + \sqrt{(n-2)^2 + 16}}{2}.$$

Now if $G \neq G_1$, then we consider the following two cases

Case I: G has at most $\binom{n}{2} - 3$ edges. In this case there are principal submatrices of $\mathcal{D}(G)$ of order $n-1$ which dominates M . Therefore we get

$$\rho_2(G) > \rho(M) = \frac{n-2 + \sqrt{(n-2)^2 + 16}}{2}.$$

Case II: If $G = G_2$, then it can be observed that $\rho_2(G_2) = \rho(A)$, where

$$A = \begin{pmatrix} 0 & 2 & 2 & \mathbb{I} \\ 2 & 0 & 1 & 1 \\ 2 & 1 & 0 & \mathbb{I} \\ \mathbb{I} & \mathbb{I} & \mathbb{I} & \mathbb{J} - I \end{pmatrix}.$$

If (ρ, x) is the eigenpair of A , then due to symmetry,

$$x_2 = x_3 \text{ and } x_4 = x_5 = \cdots = x_n.$$

Therefore from eigenequations we have

$$2x_2 + 2x_2 + (n-4)x_4 = \rho x_1 \quad (3.21)$$

$$2x_1 + x_2 + (n-4)x_4 = \rho x_2 \quad (3.22)$$

$$x_1 + 2x_2 + (n-5)x_4 = \rho x_4 \quad (3.23)$$

From (3.21)-(3.23), we have

$$\begin{vmatrix} \rho & -4 & -(n-4) \\ -2 & \rho-1 & -(n-4) \\ -1 & -2 & \rho-n+5 \end{vmatrix} = 0$$

Which implies $(\rho+2)[\rho^2 - (n-1)\rho + (n-8)] = 0$

Therefore $\rho(A)$ is the largest root of $y^2 - (n-1)y + n-8 = 0$.

Let

$$f(y) = y^2 - (n-1)y + n-8.$$

Then it can be verified that

$$f\left(\frac{n-2 + \sqrt{(n-2)^2 + 16}}{2}\right) = \frac{n - \sqrt{n^2 - 4n + 20}}{2} - 3.$$

Now $G \neq K_n, K_n - e$ gives $n \geq 4$. Which in turn implies that



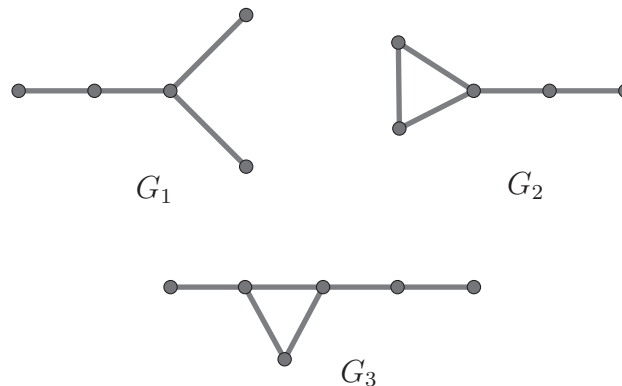


Fig. 1 Graphs with maximum number of distance Pareto eigenvalues of order 5 and 6

$$\frac{n-2+\sqrt{(n-2)^2+16}}{2} < 3$$

$$\text{Thus } f\left(\frac{n-2+\sqrt{(n-2)^2+16}}{2}\right) < 0$$

Hence the largest root of $f(y) = 0$ must be greater than $\frac{n-2+\sqrt{(n-2)^2+16}}{2}$.
i.e.

$$\rho_2(G) \geq \frac{n-2+\sqrt{(n-2)^2+16}}{2},$$

with equality if and only if $G = G_1$. □

Theorem 3.9 If $\lambda_2(G)$ is the second largest distance eigenvalue of a connected graph G , then $\rho_2(G) > \lambda_2(G)$.

Proof Let

$$D(G) = \begin{pmatrix} 0 & \mathbf{x}^T \\ \mathbf{x} & B \end{pmatrix} \text{ such that } \rho_2(G) = \rho(B).$$

From Cauchy's inequality (Lemma 2.4), we have

$$\rho_2(G) \geq \lambda_2(G),$$

with equality if and only if there exists $z \in \mathbb{C}^{n-1} - \{\mathbf{0}\}$ such that

$$Bz = \rho(B)z \text{ and } \mathbf{x}^T z = 0.$$

Here $\mathbf{x}$ is always a positive vector and z being an eigenvector corresponding to the Perron value of a nonnegative irreducible matrix is real and is either positive or negative. In either case $\mathbf{x}^T z = 0$ can never hold. Hence $\rho_2(G) > \lambda_2(G)$. □

Theorem 3.10 If G and $G' = G - e$ are connected graphs, then $\rho_2(G') \geq \rho_2(G)$.

Proof Suppose $\rho_2(G) = \rho(A)$, where A is the submatrix of $D(G)$ obtained by deleting row and column of $D(G)$ corresponding to vertex $v \in G$. Let B be the submatrix of $D(G')$ obtained by deleting row and column corresponding to vertex v .

Then clearly either $B = A$ or B dominates A . Thus $\rho_2(G') \geq \rho_2(G)$. □

Note: The inequality in Theorem 3.10 is not always strict. For example we can consider the graphs G_1 and $G_2 = G_1 - e$ as in Figure 2 with $\rho_2(G_1) = 6 = \rho_2(G_2)$. In Theorem 3.10 if e is not incident with v then



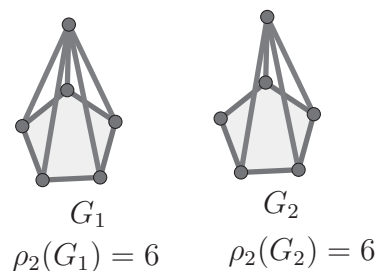


Fig. 2 Graphs G_1 and $G_2 = G_1 - e$ with $\rho_2(G_1) = \rho_2(G_2)$.

clearly B dominates A and therefore $\rho_2(G') > \rho_2(G)$. Besides if e connects v to $u \in V(G)$ and for some $i, j (\neq v) \in V(G)$, if d_{ij} increases from G to G' then again B dominates A and therefore $\rho_2(G') > \rho_2(G)$. In this regard the problem of classifying the edges (if any) in a graph G whose removal do not increase $\rho_2(G)$ seems to be an interesting problem.

From Theorem 3.10 we get the following result as immediate corollary.

Corollary 3.11 *Among all connected graphs of given order, second largest distance Pareto eigenvalue is maximum for some tree.*

Lemma 3.12 *If $a \leq b$, then $\rho_2(K_{a,b}) = a + b - 3 + \sqrt{a^2 + b^2 + b - ab - 2a + 1}$.*

Proof If $a = 1$ then by Lemma 2.20 we know that $\rho_2(K_{a,b}) = 2(b - 1)$. Now if $a \geq 2$ then up to permutation similarity $\mathcal{D}(K_{a,b})$ has exactly two distinct principal submatrices of order $n - 1$ namely $\mathcal{D}(K_{a-1,b})$ and $\mathcal{D}(K_{a,b-1})$. It can be observed that

$$\rho_1(K_{a,b}) = a + b - 2 + \sqrt{a^2 + b^2 - ab}.$$

Therefore we get

$$\begin{aligned} & \rho(\mathcal{D}(K_{a-1,b})) \\ & \quad + \sqrt{a^2 + b^2 + b - ab - 2a + 1} \text{ and} \\ \rho(\mathcal{D}(K_{a,b-1})) & = a + b - 3 \\ & \quad + \sqrt{a^2 + b^2 + a - ab - 2b + 1} \end{aligned}$$

Now $a \leq b$ implies that $\rho(\mathcal{D}(K_{a-1,b})) > \rho(\mathcal{D}(K_{a,b-1}))$ and the lemma follows. $\square$

Theorem 3.13 *If G is a connected bipartite graph of order n , then*

$$\rho_2(G) \geq n - 3 + \sqrt{n^2 + n + 1 + 3 \left\lfloor \frac{n}{2} \right\rfloor \left(\left\lfloor \frac{n}{2} \right\rfloor - n - 1 \right)}$$

equality is attained if and only if $G = K_{\lfloor \frac{n}{2} \rfloor, \lceil \frac{n}{2} \rceil}$

Proof Let G be a bipartite graph with $V(G) = V_1 \cup V_2$ as vertex bipartition such that $|V_1| = p$ and $|V_2| = q$. Then from Theorem 3.10 we have

$$\rho_2(G) \geq \rho_2(K_{p,q}). \quad (3.24)$$

Now from the proof of Lemma 3.12 we see that for any edge $e = (u, v)$ in $K_{p,q}$, where $p \geq 2$ we can have a vertex w in $K_{p,q}$ different from u and v so that $\rho_2(K_{p,q}) = \rho(A)$ where $A = (\mathcal{D}(K_{p,q}))(w)$. Since e is not incident with w , therefore $(\mathcal{D}(K_{p,q} - e))(w)$ dominates A and therefore $\rho_2(K_{p,q} - e) > \rho(K_{p,q})$. Thus equality in (3.24) holds if and only if $G = K_{p,q}$. Again for $p \leq \lfloor \frac{n}{2} \rfloor$ writin $q = n - p$ we get from Lemma 3.12

$$\rho_2(K_{p,n-p}) = n - 3 + \sqrt{n^2 + n + 1 + 3p(p - n - 1)}$$

which is a strictly decreasing function for $p \leq \lfloor \frac{n}{2} \rfloor$. Thus we get

$$\rho_2(K_{1,n-1}) > \rho_2(K_{2,n-2}) > \cdots > \rho_2(K_{\lfloor \frac{n}{2} \rfloor, \lceil \frac{n}{2} \rceil})$$



Considering all the above arguments we can say that $\rho_2(G) \geq \rho_2(K_{[\frac{q}{2}], [\frac{q}{2}]})$ and equality holds if and only if $G = K_{[\frac{q}{2}], [\frac{q}{2}]}$. This proves the theorem. $\square$

Lemma 3.14 *Let G be a tree, G' be any connected graph and $G^v = G_v * G'_w$ with $v \in V(G)$, $w \in V(G')$ and $\rho^u(G^v) = \rho(A_u)$ where $A_u = \mathcal{D}(G^v)(u)$. If $i, j, k \in V(G)$ with $i \sim j \sim k$ then for any $u \in V(G) \cup V(G')$*

$$\rho^u(G^i) + \rho^u(G^k) \geq 2\rho^u(G^j).$$

Furthermore, either $\rho^u(G^i) > \rho^u(G^j)$ or $\rho^u(G^k) > \rho^u(G^j)$.

Proof Without loss of generality we have

$$\mathcal{D}(G^i) + \mathcal{D}(G^k) - 2\mathcal{D}(G^j) = \begin{pmatrix} G' & G_i & G_j & G_k \\ 0 & 0 & 2\mathbb{J} & 0 \\ 0 & 0 & 0 & 0 \\ 2\mathbb{J}^T & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}$$

where G_i, G_j, G_k are components of $G - \{ij, jk\}$ containing i, j, k respectively. Now since $|V(G_i)| \geq 1$ and $|V(G')| \geq 2$, for any $u \in V(G) \cup V(G')$ we get

$$\mathcal{D}(G^i)(u) + \mathcal{D}(G^k)(u) - 2\mathcal{D}(G^j)(u) \geq 0.$$

Therefore if $\mathbf{x}$ is the Perron vector of $\mathcal{D}(G^j)(u)$, then

$$\mathbf{x}^T \{\mathcal{D}(G^i)(u) + \mathcal{D}(G^k)(u) - 2\mathcal{D}(G^j)(u)\} \mathbf{x} \geq 0$$

Thus from Fig. 3 we have

$$\begin{aligned} & \rho^u(G^i) + \rho^u(G^k) - 2\rho^u(G^j) \\ & \geq \rho(\mathcal{D}(G^i)(u) + \mathcal{D}(G^k)(u) - 2\mathcal{D}(G^j)(u)) \\ & \geq \mathbf{x}^T \{\mathcal{D}(G^i)(u) + \mathcal{D}(G^k)(u) - 2\mathcal{D}(G^j)(u)\} \mathbf{x} \\ & \geq 0. \end{aligned} \tag{3.25}$$

Now if $|V(G_i)| \geq 2$ or if $u \neq j$, then $\mathcal{D}(G^i)(u) + \mathcal{D}(G^k)(u) - 2\mathcal{D}(G^j)(u) \neq 0$ and therefore Inequality (3.25) is strict and we are done. But if $u = j$, then $\mathcal{D}(G^i)(u) + \mathcal{D}(G^k)(u) - 2\mathcal{D}(G^j)(u) = 0$. In this case to the contrary we assume that $\rho^u(G^i) = \rho^u(G^k) = \rho^u(G^j) = \rho$ (say). Then we must have $\mathcal{D}(G^i)(u)\mathbf{x} = \rho\mathbf{x}$, $\mathcal{D}(G^j)(u)\mathbf{x} = \rho\mathbf{x}$ and $\mathcal{D}(G^k)(u)\mathbf{x} = \rho\mathbf{x}$. But we see that

$$\mathcal{D}(G^i)(u) - \mathcal{D}(G^j)(u) = \begin{pmatrix} G' & G_i & G_k \\ 0 & -\mathbb{J} & \mathbb{J} \\ -\mathbb{J}^T & 0 & 0 \\ \mathbb{J}^T & 0 & 0 \end{pmatrix}$$

Therefore as $(\mathcal{D}(G^i)(u) - \mathcal{D}(G^j)(u))\mathbf{x} = 0$ we observe from the above matrix that

$$\sum_{\ell \in V(G_i)} x_\ell = 0 \text{ and } \sum_{\ell \in V(G_k)} x_\ell = 0$$

which are not possible as $\mathbf{x}$ is a positive vector and $V(G_i)$, $V(G_k)$ are non empty. Hence either $\rho^u(G^i) \neq \rho^u(G^j)$ or $\rho^u(G^k) \neq \rho^u(G^j)$ and therefore we get the result as desired. $\square$

Corollary 3.15 *Let T be a tree and G' be a graph. Then $\rho_2(G^i)$ is strictly quasiconvex on T , where G^i is as defined in Lemma 3.14.*

Proof Let u be the vertex of G^j , so that $\rho_2(G^j) = \rho(\mathcal{D}(G^j)(u))$. Then by Lemma 3.14, we get either $\rho^u(G^i) > \rho_2(G^j)$ or $\rho^u(G^k) > \rho_2(G^j)$. But by Theorem 3.1 we have $\rho_2(G^i) \geq \rho^u(G^i)$ and $\rho_2(G^k) \geq \rho^u(G^k)$. Hence the result follows. $\square$



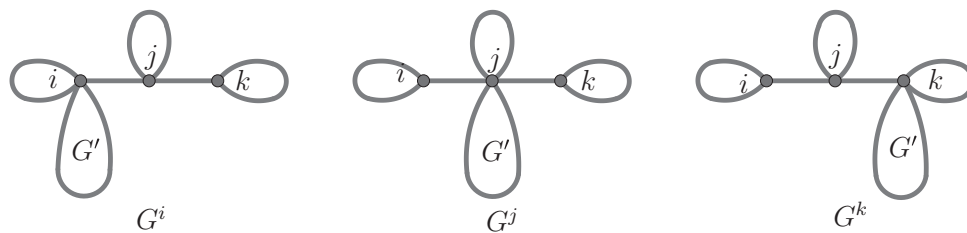


Fig. 3 Graphs G^i, G^j, G^k in Lemma 3.14

As a result of repeated application of Lemma 2.12 and Corollary 3.15 we get the following results.

Theorem 3.16 *Among all trees of given order, the second largest distance Pareto eigenvalue is maximized in the path graph.*

Theorem 3.17 *Among all trees of given order, the second largest distance Pareto eigenvalue is minimized in the star graph.*

From Theorem 2.22 we see that among all connected graphs of given order n the minimum value of the second largest distance Pareto eigenvalue is $n - 2$ and is uniquely achieved by the complete graph K_n . Now using Corollary 3.11 and Theorem 3.16 we have the following result regarding the unique graph with maximum second largest distance Pareto eigenvalue among all connected graphs of given order.

Theorem 3.18 *Among all connected graphs of given order, the second largest distance Pareto eigenvalue is maximized in the path graph.*

Let us reserve the following notations for the rest of this article. For $S \subset [n]$,

$$X_n(S) = \{\mathbf{x} \in \mathbb{R}^n : \mathbf{x} \geq 0, \mathbf{x}^T \mathbf{x} = 1, \mathbf{x}_i = 0 \Leftrightarrow i \in S\}$$

and $X_n^k = \{\mathbf{x} \in X_n(S) : S \subset [n], |S| = k\}.$

Theorem 3.19 *If $A \in M_n$ is symmetric, nonnegative and irreducible (or positive), then*

$$\rho_2(A) = \max_{\mathbf{x} \in X_n^1} \mathbf{x}^T A \mathbf{x}.$$

Proof From Theorem 2.8, it can be observed that $\rho_2(A)$ is the largest possible eigenvalue among all principal submatrices of A of order $n - 1$.

For any $i \in [n]$ let $B_i = A(i)$ and $\mathbf{x} \in \mathbb{R}^{n-1}$ be an arbitrary normalized vector. If we take $\mathbf{z} \in \mathbb{R}^n$ such that $z_i = 0$ and $z_j = \mathbf{x}_j$ for $j \neq i$, then $\mathbf{z}^T A \mathbf{z} = \mathbf{x}^T B_i \mathbf{x}$. Now

$$\begin{aligned} \rho(B_i) &= \max_{\substack{\mathbf{x} \in \mathbb{R}^{n-1} \\ \mathbf{x}^T \mathbf{x} = 1}} \mathbf{x}^T B_i \mathbf{x} \\ &= \max_{\mathbf{x} \in X_{n-1}^0} \mathbf{x}^T B_i \mathbf{x} \\ &= \max_{\mathbf{z} \in X_n(\{i\})} \mathbf{z}^T A \mathbf{z} \end{aligned}$$

Therefore
$$\begin{aligned} \rho_2(A) &= \max_{i \in [n]} \rho(B_i) \\ &= \max_{i \in [n]} \max_{\mathbf{z} \in X_n(\{i\})} \mathbf{z}^T A \mathbf{z} \\ &= \max_{\substack{\mathbf{z} \in X_n(\{i\}) \\ i \in [n]}} \mathbf{z}^T A \mathbf{z} \\ &= \max_{\mathbf{z} \in X_n^1} \mathbf{z}^T A \mathbf{z} \end{aligned}$$

This completes the proof. □

Corollary 3.20 If $z \in X_n^1$ and $A \in M_n$ is symmetric, nonnegative irreducible (or positive) then

$$\min_{z \in X_n^1} z^T A z \leq \rho_2(A) \leq \max_{z \in X_n^1} z^T A z,$$

with left hand (right hand) equality if and only if z is the normalized Pareto eigenvector of A corresponding to $\rho_2(A)$.

Corollary 3.21 If $A \in M_n$ is symmetric, nonnegative irreducible (or positive) then

$$\rho_2(A) = \max_{x \in T_n^1} \frac{x^T A x}{x^T x}$$

where $T_n^k = \{x \in \mathbb{R}^n : x \geq 0 \text{ and } x_i = 0 \text{ for exactly } k \text{ values of } i \in [n]\}$.

Theorem 3.22 If G is a connected graph of diameter d and $T_{\min} = \min_{v \in V(G)} \text{Tr}(v)$, then

$$\rho_2(G) \geq \frac{T_{\min} - 2d + \sqrt{(T_{\min} - 2d)^2 + 4(n - d - 1)}}{2}$$

Equality holds if and only if $G = K_n$.

Proof Let $\mathbf{x} = (x_1, x_2, \dots, x_n)^T$ be the Pareto eigenvector of $\mathcal{D}(G)$ corresponding to $\rho_2(G)$ with $x_i = 0$ i.e. $\rho_2(G) = \rho(\mathcal{D}(G)(i))$.

Let

$$x_j = \min_{\ell \neq i} x_\ell \text{ and } x_k = \min_{\ell \neq i, j} x_\ell.$$

For $j \in V(G)$ if $T_j = \text{Tr}(j)$, then from Pareto eigenequations we have

$$\rho_2 x_j = \sum_{\ell \in V(G)} d_{j\ell} x_\ell \tag{3.26}$$

$$\geq (T_j - d_{ji})x_k \tag{3.27}$$

$$\begin{aligned} \rho_2 x_k &= \sum_{\ell \in V(G)} d_{k\ell} x_\ell \\ &\geq d_{kj}x_j + (T_k - d_{ki} - d_{kj})x_k \\ &\geq x_j + (T_k - 2d)x_k \end{aligned} \tag{3.28}$$

From (3.27) and (3.28) we get

$$\begin{aligned} \rho_2(\rho_2 - T_k + 2d) - T_j + d &\geq 0 \\ \Rightarrow \rho_2 &\geq \frac{T_k - 2d + \sqrt{(T_k - 2d)^2 + 4(T_j - d)}}{2} \\ &\geq \frac{T_k - 2d + \sqrt{(T_k - 2d)^2 + 4(n - d - 1)}}{2}. \end{aligned} \tag{3.29}$$

If $G = K_n$, then $T_k = n - 1$ and $d = 1$. Therefore by Lemma 2.16 equality holds in (3.29).

Now suppose the equality holds in (3.29) then equality must hold in all the inequalities (3.26)-(3.29). Equality in (3.29) gives $d_j = n - 1$. Again equality in (3.28) implies $d_{jk} = d$. Therefore we must have $d = 1$ i.e. $G = K_n$. $\square$



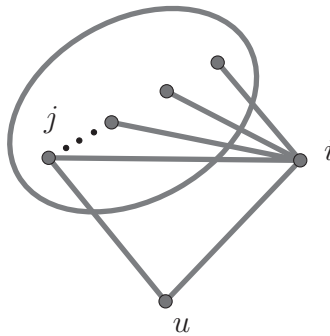


Fig. 4 Graph $H_{i,u}$ as in Theorem 3.23

Theorem 3.23 Let G is a connected graph and $(\rho_2(G), \mathbf{x})$ be a distance Pareto eigenpair of G . If the second largest component of $\mathbf{x}$ corresponds to $j \in V(G)$ then

$$\rho_2(G) \leq \frac{T_j - 2 + \sqrt{(T_j - 2)^2 + 4(n - 2)}}{2}.$$

If equality holds, then $G \cong H_{u,v}$ for some $u, v \in V(G)$.

Proof Let $\mathbf{x} = (x_1, x_2, \dots, x_n)^T$ be the Pareto eigenvector of $\mathcal{D}(G)$ corresponding to $\rho_2(G)$ with $x_u = 0$ i.e. $\rho_2(G) = \rho(\mathcal{D}(G)(u))$.

Let

$$x_i = \max_{k \in [n]} x_k \text{ and } x_j = \max_{k \neq i} x_k$$

From Pareto eigenequations we have

$$\begin{aligned} \rho_2 x_i &= \sum_{\ell \in V(G)} d_{i\ell} x_\ell \\ &\leq (T_i - d_{iu}) x_j \\ &\leq (T_i - 1) x_j \end{aligned} \quad (3.30)$$

and

$$\begin{aligned} \rho_2 x_j &\leq d_{ij} x_i + (T_j - d_{ju} - d_{ij}) x_j \\ &\leq x_i + (T_j - 2) x_j \end{aligned} \quad (3.31)$$

Now (3.30) and (3.31) together implies $\rho_2^2 - (T_j - 2)\rho_2 - (T_i - 1) \leq 0$. Which in turn gives

$$\rho_2 \leq \frac{T_j - 2 + \sqrt{(T_j - 2)^2 + 4(n - 2)}}{2} \quad (3.32)$$

Now suppose the equality holds in (3.32), then equality must hold in (3.30) and (3.31) as well.

Equality in (3.30) implies

$$\begin{aligned} i \sim u \text{ and } x_k &= x_j \text{ for all } k \neq i, u \\ \text{Thus } T_k &= T_j \text{ for all } k \neq i, u \\ &[\text{using (3.31)}] \end{aligned} \quad (3.33)$$

Equality in (3.31) implies $i \sim j \sim u$ and equality in (3.32) gives $d_i = n - 1$ and so $\text{diam}(G) \leq 2$. Hence using (3.33) we get $T_k = d_k + 2(n - d_k - 1) = 2(n - 1) - d_k$ for all $k \neq i, u$.

Combining all the above arguments, we get the required result (Fig. 4). $\square$

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