MATEMATIČKI VESNIK
МАТЕМАТИЧКИ ВЕСНИК
76, 1–2 (2024), 29–42
March 2024

research paper
оригинални научни рад
DOI: 10.57016/MV-vJ5201ZF

ON THE GENERALIZED DISTANCE EIGENVALUES OF GRAPHS

A. Alhevaz, M. Baghipur, H. A. Ganie and K. C. Das

Abstract. For a simple connected graph G, the generalized distance matrix $D_\alpha(G)$ is defined as $D_\alpha(G) = \alpha Tr(G) + (1-\alpha)D(G),\ 0 \leq \alpha \leq 1$. The largest eigenvalue of $D_\alpha(G)$ is called the generalized distance spectral radius or D_α-spectral radius of G. In this paper, we obtain some upper bounds for the generalized distance spectral radius in terms of various graph parameters associated with the structure of graph G, and characterize the extremal graphs attaining these bounds. We determine the graphs with minimal generalized distance spectral radius among the trees with given diameter d and among all unicyclic graphs with given girth. We also obtain the generalized distance spectrum of the square of the cycle and the square of the hypercube of dimension n. We show that the square of the hypercube of dimension n has three distinct generalized distance eigenvalues.

1. Introduction

All graphs considered here are simple, undirected and connected. Let G be a graph with vertex set $V(G) = \{v_1, v_2, \ldots, v_n\}$ and edge set $E(G)$. The *order* of G is the number $n = |V(G)|$ and its *size* is the number $|E(G)|$. The set of vertices adjacent to $v \in V(G)$, denoted by $N(v)$, is the *neighborhood* of v. The *degree* of v, denoted by $d_G(v)$ (we simply write d_v if it is clear from the context) means the cardinality of $N(v)$. A graph is called *regular* if each of its vertices has the same degree. The *distance* between two vertices $u, v \in V(G)$, denoted by d_{uv}, is defined as the length of the shortest path between u and v in G. The *diameter* of G is the maximum distance between any two vertices of G. The *distance matrix* of G is denoted $D(G)$ and is defined as $D(G) = (d_{uv})_{u,v \in V(G)}$. For some spectral properties of the distance matrix of graphs, we refer the reader to the survey [9]. The *transmission* $Tr_G(v)$ of a vertex v is defined as the sum of the distances from v to all other vertices in G, i.e. $Tr_G(v) = \sum_{u \in V(G)} d_{uv}$. A graph G is called *k-transmission regular* if $Tr_G(v) = k$, for every $v \in V(G)$. The *transmission* (also called *Wiener index*) of a graph G, denoted

2020 Mathematics Subject Classification: 05C50, 05C12, 15A18
Keywords and phrases: Generalized distance matrix (spectrum); spectral radius; hypercube; unicyclic graph.

by $W(G)$, is the sum of the distances between all unordered pairs of vertices in G. Obviously, $W(G) = \frac{1}{2}\sum_{v\in V(G)} Tr_G(v)$. For each vertex $v_i \in V(G)$, the transmission $Tr_G(v_i)$ is also called *transmission degree*, denoted Tr_i for short, and the sequence $\{Tr_1, Tr_2, \ldots, Tr_n\}$ is called *transmission degree sequence* of the graph G. The *second transmission* of v_i, denoted by T_i is given by $T_i = \sum_{j=1}^{n} d_{ij} Tr_j$, where $d_{ij} = d_{v_i v_j}$.

Let $Tr(G) = diag(Tr_1, Tr_2, \ldots, Tr_n)$ be the diagonal matrix of vertex transmissions of G. M. Aouchiche and P. Hansen [10, 11] introduced the Laplacian and the signless Laplacian for the distance matrix of a connected graph. The matrix $D^L(G) = Tr(G) - D(G)$ is called the *distance Laplacian matrix* of G, while the matrix $D^Q(G) = Tr(G) + D(G)$ is called the *distance signless Laplacian matrix* of G. The spectral properties of $D(G)$, $D^L(G)$ and $D^Q(G)$ have attracted the attention of researchers, and a large number of papers have been published on their spectral properties, such as spectral radius, second largest eigenvalue, smallest eigenvalue, etc. For some recent works, we refer to [2, 7, 10–12] and the references therein.

Cui et al. [15] introduced the *generalized distance matrix* $D_\alpha(G)$ as a convex combination of $Tr(G)$ and $D(G)$, defined as $D_\alpha(G) = \alpha Tr(G) + (1-\alpha)D(G)$, for $0 \le \alpha \le 1$. Since $D_0(G) = D(G)$, $2D_{\frac{1}{2}}(G) = D^Q(G)$, $D_1(G) = Tr(G)$, and $D_\alpha(G) - D_\beta(G) = (\alpha - \beta)D^L(G)$, each result concerning the spectral properties of the generalized distance matrix has its counterpart for each of these particular graph matrices, and these counterparts follow directly from a single proof. In fact, this matrix reduces to merging the distance spectral and the distance signless Laplacian spectral theories. Since the matrix $D_\alpha(G)$ is real symmetric, all its eigenvalues are real. Therefore, we can arrange them as $\partial_1 \ge \partial_2 \ge \cdots \ge \partial_n$. The largest eigenvalue ∂_1 of the matrix $D_\alpha(G)$ is called the *generalized distance spectral radius* of G (from now on we denote $\partial_1(G)$ by $\partial(G)$). Since $D_\alpha(G)$ is non-negative and irreducible (except for $\alpha = 1$), by the Perron-Frobenius theorem $\partial(G)$ is the unique eigenvalue, and there is a unique positive unit eigenvector X corresponding to $\partial(G)$, which is called the *generalized distance Perron vector* of G. For some recent results concerning the generalized distance matrix (spectrum) of graphs, we refer the reader to the papers [1, 3–6, 8, 15, 17, 18, 21, 23].

A column vector $X = (x_1, x_2, \ldots, x_n)^T \in \mathbb{R}^n$ can be viewed as a function defined on $V(G)$ which maps vertex v_i to x_i, i.e., $X(v_i) = x_i$ for $i = 1, 2, \ldots, n$. Then, $X^T D_\alpha(G) X = \alpha \sum_{i=1}^{n} Tr(v_i)x_i^2 + 2(1-\alpha)\sum_{1\le i<j\le n} d(v_i, v_j)x_i x_j$, and λ is an eigenvalue of $D_\alpha(G)$ corresponding to the eigenvector X if and only if $X \neq \mathbf{0}$ and

$$\lambda x_{v_i} = \alpha Tr(v_i)x_i + (1-\alpha)\sum_{j=1}^{n} d(v_i, v_j)x_j.$$

These equations are called the (λ, x)-*eigenequations* of G. For a normalized column vector $X \in \mathbb{R}^n$ with at least one nonnegative component, by the Rayleigh's principle, we have $\partial(G) \ge X^T D_\alpha(G) X$, with equality if and only if X is the generalized distance Perron vector of G.

The rest of the paper is organized as follows. In Section 2 we mention some preliminary results that will be useful in the rest of the paper. In Section 3, we obtain some upper bounds on the generalized distance spectral radius $\partial(G)$ as a function of various graph parameters associated with the structure of the graph G, and characterize the extremal graphs attaining these bounds. In Section 4, we determine the graphs with minimum generalized distance spectral radius among trees of given diameter d and among all unicyclic graphs of given girth. In Section 5, we obtain the generalized distance spectrum of the square of the cycle and the square of the hypercube of dimension n. We show that the square of the hypercube of dimension n has three distinct generalized distance eigenvalues.

2. Preliminary results

In this section we give some already known results which will be needed in the sequel. The following lemma can be found in [15].

Lemma 2.1 ([15]). *Let G be a connected graph of order n. Then, $\partial(G) \geq \frac{2W(G)}{n}$, with equality if and only if G is a transmission regular graph.*

Lemma 2.2 ([13]). *Let B be a nonnegative irreducible matrix with row sums $r_1, r_2, \ldots, r_n$. If $\mu(B)$ is the largest eigenvalue of B, then $\min_{1 \leq i \leq n} r_i \leq \mu(B) \leq \max_{1 \leq i \leq n} r_i$, with each equality if and only if $r_1 = r_2 = \cdots = r_n$.*

Lemma 2.3 ([14, Interlacing theorem]). *Let A be a symmetric real matrix and B be a principal submatrix of A of order n and s ($s \leq n$), respectively. Then, for the eigenvalues of A and B, $\lambda_{i+n-s}(A) \leq \lambda_i(B) \leq \lambda_i(A)$, $1 \leq i \leq s$.*

Lemma 2.4 ([14, Courant-Weyl inequality]). *Let A_1 and A_2 be symmetric real matrices of order n. For $1 \leq i \leq n$, satisfy the eigenvalues of A_1 and A_2: $\lambda_n(A_2)+\lambda_i(A_1) \leq \lambda_i(A_1 + A_2) \leq \lambda_i(A_1) + \lambda_1(A_2)$.*

Obviously, $D_\alpha(G)$ is a symmetric real matrix, hence by Lemma 2.3 the following corollary follows immediately.

Corollary 2.5. *Let G be a graph of order n. Let M be the principal submatrix of $D_\alpha(G)$ of order $n-1$. Then, $\partial_1(G) \geq \lambda_1(M) \geq \partial_2(G) \geq \ldots \geq \lambda_{n-1}(M) \geq \partial_n(G)$.*

Lemma 2.6 ([15]). *Let G be a connected graph of order n and $\frac{1}{2} \leq \alpha \leq 1$. If G' is a connected graph obtained from G by deleting an edge, then for every $1 \leq i \leq n$, $\partial(G') \geq \partial(G)$.*

Lemma 2.7 ([24]). *If $x_1 \geq x_2 \geq \cdots \geq x_m$ are real numbers such that $\sum_{i=1}^m x_i = 0$, then $x_1 \leq \sqrt{\frac{m-1}{m} \sum_{i=1}^m x_i^2}$. The equality holds if and only if $x_2 = \cdots = x_m = -\frac{x_1}{m-1}$.*

The proof of the following lemma is similar to that of [19, Lemma 2] and is therefore omitted here.

Lemma 2.8 ([19]). *A connected graph G has two distinct $D_\alpha(G)$-eigenvalues if and only if G is a complete graph.*

3. Bounds on spectral radius of the generalized distance matrix

In this section we obtain upper bounds for the generalized distance spectral radius of a connected graph G, in terms of various graph parameters associated with the structure of the graph. We characterize the extremal graphs that reach these bounds.

The following result gives an upper bound for the generalized distance spectral radius of a graph.

THEOREM 3.1. *Let G be a graph of order n with maximum transmission degree $Tr_{\max}$. Then $\partial(G) < \alpha Tr_{\max} + (1-\alpha)\sqrt{2\sum_{1\le i<j\le n} d_{ij}^2 + \frac{3}{n}\sum_{i=1}^n Tr_i^2}$.*

Proof. Let $X = (x_1, x_2, \ldots, x_n)^T$ be a unit eigenvector corresponding to $\partial(G)$ of the generalized distance matrix $D_\alpha(G)$ of G. Then we have $D_\alpha(G)X = \partial X$. For $v_i \in V(G)$, we have

$$\partial(G)x_i = \alpha Tr_i x_i + (1-\alpha)\sum_{j=1}^n d_{ij}x_j,$$

that is

$$(\partial(G) - \alpha Tr_i)^2 x_i^2 = (1-\alpha)^2\left(\sum_{j=1}^n d_{ij}x_j\right)^2. \tag{1}$$

As $\sum_{i=1}^n x_i^2 = 1$ and $\sum_{i=1}^n x_i = 1$, then by Cauchy-Schwarz inequality, we have

$$\begin{aligned}\left(\sum_{j=1}^n d_{ij}x_j\right)^2 &< \left(\sum_{j=1}^n x_j\left(d_{ij} + \frac{Tr_i}{n}\right)\right)^2\\ &\le \sum_{j=1}^n x_j^2 \sum_{j=1}^n\left(d_{ij}^2 + \left(\frac{Tr_i}{n}\right)^2 + \frac{2d_{ij}Tr_i}{n}\right) = \sum_{j=1}^n d_{ij}^2 + \frac{3Tr_i^2}{n}.\end{aligned}$$

Then

$$\sum_{i=1}^n\left(\sum_{j=1}^n d_{ij}x_j\right)^2 < 2\sum_{1\le i<j\le n} d_{ij}^2 + \frac{3}{n}\sum_{i=1}^n Tr_i^2.$$

Using (1) with the above result, we have

$$(\partial(G)-\alpha Tr_{\max})^2 \le \sum_{i=1}^n(\partial(G)-\alpha Tr_i)^2 x_i^2 < (1-\alpha)^2\left(2\sum_{1\le i<j\le n} d_{ij}^2 + \frac{3}{n}\sum_{i=1}^n Tr_i^2\right).$$

Thus, the result follows. □

The following observations follow directly from Theorem 3.1.

COROLLARY 3.2. *If G is a connected graph of order n and diameter d, then $\partial(G) < \frac{\alpha n(n-1)}{2} + (1-\alpha)\sqrt{(n-1)(nd^2+3n-3)}$.*

Proof. Since $d_{ij} \leq d$ for $i \neq j$ and there are $\frac{n(n-1)}{2}$ pairs of vertices in G, we obtain from Theorem 3.1

$$\begin{aligned}\partial(G) &< \frac{\alpha n(n-1)}{2} + (1-\alpha)\sqrt{2\frac{n(n-1)}{2}d^2 + \frac{3}{n}n(n-1)^2} \\ &= \frac{\alpha n(n-1)}{2} + (1-\alpha)\sqrt{(n-1)\left(nd^2 + 3n - 3\right)}.\end{aligned}$$

□

COROLLARY 3.3. *Let G be a connected k-transmission graph of order n. Then* $\partial(G) < \alpha k + (1-\alpha)\sqrt{2\sum_{1\leq i<j\leq n} d_{ij}^2 + 3k^2}$.

The following result gives another upper bound for the generalized distance spectral radius $\partial(G)$, in terms of transmission degrees and the parameter α.

THEOREM 3.4. *Let G be a graph of order n, where $n \geq 2$. If $Tr_1 \geq \ldots \geq Tr_n$ and $Tr_1 > Tr_{n-k+1}$, for a fixed integer k, $1 \leq k \leq n-1$, then*

$$\begin{aligned}\partial(G) \leq{}& \frac{\alpha Tr_{n-k+1} + Tr_1 + \alpha - 1}{2} \\ &+ \frac{\sqrt{\left(Tr_1 - \alpha Tr_{n-k+1} - (1-\alpha)(2k-1)\right)^2 + 4(1-\alpha)^2(Tr_{n-k+1} - k + 1)}}{2}, \qquad (2)\end{aligned}$$

with equality holding if and only if G is a graph with k ($k \leq n-2$) vertices of degree $n-1$ and the remaining $n-k$ vertices have equal degree less than $n-1$.

Proof. Let G be a connected graph with vertex set $V(G) = \{v_1, v_2, \ldots, v_n\}$. Let $V_1 = \{v_1, \ldots, v_{n-k}\}$ and $V_2 = V(G)\backslash V_1$. Then $D_\alpha(G) = M + N$ may be partitioned as

$$M = (1-\alpha)\begin{pmatrix} D_{11} & D_{12} \\ D_{21} & D_{22}\end{pmatrix}, \quad N = \alpha\begin{pmatrix} Tr_{11} & 0 \\ 0 & Tr_{22}\end{pmatrix},$$

where D_{11} and Tr_{11} are $(n-k)\times(n-k)$ matrices. Let

$$U = \begin{pmatrix} \frac{1}{x}I_{n-k} & 0 \\ 0 & I_k\end{pmatrix}$$

for $0 < x < 1$ (to be determined) and $B = U^{-1}D_\alpha(G)U = P + N$, where I_s is the $s\times s$ unit matrix and

$$P = (1-\alpha)\begin{pmatrix} D_{11} & xD_{12} \\ \frac{1}{x}D_{21} & D_{22}\end{pmatrix}$$

is a nonnegative irreducible matrix that has the same spectrum as $D_\alpha(G)$. Let r_i denote the i-th row sum of B. If $i = 1, 2, \ldots, n-k$, then since $d_{ij} \geq 1$ for $j = n-k+1, \ldots, n$, we have

$$\begin{aligned} r_i &= (1-\alpha)\sum_{j=1}^{n-k} d_{ij} + x(1-\alpha)\sum_{j=n-k+1}^{n} d_{ij} + \alpha\sum_{j=1}^{n} d_{ij} \\ &= (1-\alpha)\sum_{j=1}^{n} d_{ij} + (1-\alpha)(x-1)\sum_{j=n-k+1}^{n} d_{ij} + \alpha\sum_{j=1}^{n} d_{ij}\end{aligned}$$

$$= Tr_i + (1-\alpha)(x-1)\sum_{j=n-k+1}^{n} d_{ij} \le Tr_i + (1-\alpha)(x-1)k \le Tr_1 + (1-\alpha)(x-1)k.$$

If $i = n-k+1, \dots, n-k$, then since $d_{ii} = 0$ and $d_{ij} \ge 1$ for $j = n-k+1, \dots, n$ with $i \neq j$, we have

$$\begin{aligned}
r_i &= \frac{1-\alpha}{x}\sum_{j=1}^{n-k} d_{ij} + (1-\alpha)\sum_{j=n-k+1}^{n} d_{ij} + \alpha\sum_{j=1}^{n} d_{ij} \\
&= \frac{\alpha(x-1)+1}{x}\sum_{j=1}^{n} d_{ij} + (1-\alpha)\left(1-\frac{1}{x}\right)\sum_{j=n-k+1}^{n} d_{ij} \\
&= \left(\frac{\alpha(x-1)+1}{x}\right) Tr_i + (1-\alpha)\left(1-\frac{1}{x}\right)\sum_{j=n-k+1}^{n} d_{ij} \\
&\le \left(\frac{\alpha(x-1)+1}{x}\right) Tr_i + (1-\alpha)\left(1-\frac{1}{x}\right)(k-1) \\
&\le \left(\frac{\alpha(x-1)+1}{x}\right) Tr_{n-k+1} + (1-\alpha)\left(1-\frac{1}{x}\right)(k-1).
\end{aligned}$$

Let

$$\begin{aligned}
x = &\frac{\alpha Tr_{n-k+1} - Tr_1 + (1-\alpha)(2k-1)}{2(1-\alpha)k} \\
&+ \frac{\sqrt{(Tr_1 - \alpha Tr_{n-k+1} - (1-\alpha)(2k-1))^2 + 4(1-\alpha)^2(Tr_{n-k+1} - k + 1)}}{2(1-\alpha)k}.
\end{aligned}$$

Then

$$\begin{aligned}
&Tr_1 + (1-\alpha)(x-1)k = \left(\frac{\alpha(x-1)+1}{x}\right) Tr_{n-k+1} + (1-\alpha)\left(1-\frac{1}{x}\right)(k-1) \\
&= \frac{\alpha Tr_{n-k+1} + Tr_1 + \alpha - 1}{2} \\
&+ \frac{\sqrt{(Tr_1 - \alpha Tr_{n-k+1} - (1-\alpha)(2k-1))^2 + 4(1-\alpha)^2(Tr_{n-k+1} - k + 1)}}{2}.
\end{aligned}$$

Since $Tr_1 > Tr_{n-k+1} \ge Tr_n \ge n-1 > k-1$, we have $0 < x < 1$. Thus by Lemma 2.2, we have

$$\begin{aligned}
\partial(G) &\le \max_{1\le i\le n} r_i \\
&\le \frac{\alpha Tr_{n-k+1} + Tr_1 + \alpha - 1}{2} \\
&+ \frac{\sqrt{(Tr_1 - \alpha Tr_{n-k+1} - (1-\alpha)(2k-1))^2 + 4(1-\alpha)^2(Tr_{n-k+1} - k + 1)}}{2}.
\end{aligned}$$

Suppose that equality holds in (2). Since $r_i = Tr_1 + (1-\alpha)(x-1)k$ for $i = 1, 2, \dots, n-k$, we have $d_{ij} = 1$ for $i = 1, 2, \dots, n-k$ and $j = n-k+1, \dots, n$, which implies that every vertex in V_1 is adjacent to all vertices in V_2. Again, since

$r_i = \left(\frac{\alpha(x-1)+1}{x}\right) Tr_{n-k+1} + (1-\alpha)\left(1-\frac{1}{x}\right)(k-1)$ for $i = n-k+1, \ldots, n$, we have $d_{ij} = 1$ for $i, j = n-k+1, \ldots, n$ with $i \neq j$, which implies that V_2 induces a complete subgraph in G. Thus, the degree of every vertex in V_2 is $n-1$ and hence the diameter of G is at most 2. Since $Tr_1 = Tr_2 = \cdots = Tr_{n-k}$, every vertex in V_1 has the same degree. Moreover, since $Tr_1 > Tr_{n-k+1}$, G cannot be the complete graph, and thus $k \leq n-2$.

Conversely, if G is a graph stated in the second part of the theorem, then from the proof above, we have $r_1 = r_2 = \cdots = r_n$ and thus equality holds. □

The following result gives an upper bound for $\partial(G)$, in terms of Wiener index $W(G)$, the order n, the transmission degrees and the parameter α.

THEOREM 3.5. *Let G be a connected graph of order n. Then*

$$\partial(G) \leq \frac{2\alpha W(G)}{n} + \sqrt{\frac{n-1}{n}\left(2(1-\alpha)^2 \sum_{1\leq i<j\leq n} d_{ij}^2 + \alpha^2 \sum_{i=1}^{n} Tr_i^2 - \frac{4\alpha^2 W^2(G)}{n}\right)}, \quad (3)$$

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

Proof. We have $\sum_{i=1}^{n}\left(\partial_i(G) - \frac{2\alpha W(G)}{n}\right) = 0$. Applying Lemma 2.7, we get

$$\partial(G) - \frac{2\alpha W(G)}{n} \leq \sqrt{\frac{n-1}{n}\sum_{i=1}^{n}\left(\partial_i(G) - \frac{2\alpha W(G)}{n}\right)^2},$$

with equalty if and only if

$$\partial_2(G) - \frac{2\alpha W(G)}{n} = \cdots = \partial_n(G) - \frac{2\alpha W(G)}{n} = -\frac{\partial_1(G) - \frac{2\alpha W(G)}{n}}{n-1}. \quad (4)$$

Thus the inequality follows. We claim that the equality in (3) holds if and only if $G = K_n$. Suppose that the equality in (3) holds. From the equality in (4), we get $\partial_2(G) = \cdots = \partial_n(G)$. Hence the equality in (3) implies that G has only two distinct generalized distance eigenvalues, then by Lemma 2.8, $G = K_n$. Conversely, using the fact that the generalized distance eigenvalues of K_n are $\partial_1(G) = n-1$ and $\partial_i(G) = \alpha n - 1$, $i = 2, \ldots, n$, one can easily see that the equality in (3) holds. □

4. Extremal graphs for the generalized distance spectral radius for some families of graphs

In this section, we determine the graphs with minimum generalized distance spectral radius among trees of given diameter d and among all unicyclic graphs of given girth.

For a graph G, the vertices $u, v \in V(G)$ are called *multiplicate vertices* if $N_G(u) = N_G(v)$. Suppose u is adjacent to v and $N_{G-v}(u) = N_{G-u}(v)$; then u, v are called *quasi-multiplicate vertices*. In general, a subset $S \subset V(G)$ is a *multiplicate vertex set*, if $N_G(u) = N_G(v)$ for all $u, v \in S$. A subset $C \subset V(G)$ is a *quasi-multiplicate vertex* *set* if the vertices of C induce a clique and $N_G(u)-C = N_G(v)-C$ for all $u, v \in C$. It is obvious that we add edges to any two vertices of a multiplicate vertex set to obtain a quasi-multiplicate vertex set.

For two matrices $A = [a_{ij}]$ and $B = [b_{ij}]$ of order n, if $a_{ij} \leq b_{ij}$ $(1 \leq i, j \leq n)$, we say $A \leq B$ and $A < B$, if $a_{ij} < b_{ij}$ $(1 \leq i, j \leq n)$.

Theorem 4.1. *Let v be a pendent vertex of G and d be the diameter of G. Then $\partial_{i+1}(G) - \alpha d \leq \partial_i(G-v) \leq \partial_i(G) - \alpha$, for $i = 1, 2, \ldots, n-1$.*

Proof. Since v is a vertex with degree one, we get $d_{G-v}(x,y) = d_G(x,y)$ for $x, y \in V(G-v)$, and $1 \leq d_G(v,z) \leq d$ for $z \in V(G-v)$. Then $Tr_G(z) > Tr_{G-u}(z)$. Let M be the principal submatrix of $D_\alpha(G)$ obtained by deleting the row and column corresponding to v. Then $M > D_\alpha(G-v)$. Let $S = M - D_\alpha(G-v)$. Therefore $S = diag(a_1, a_2, \ldots, a_{n-1})$ where $\alpha \leq a_i \leq \alpha d$, for $i = 1, \ldots, n-1$, hence $\alpha \leq \lambda_i(S) \leq \alpha d$. Thus, by Lemma 2.4, we get

$$\partial_i(G-v) + \alpha \leq \lambda_i(M) \leq \partial_i(G-v) + \alpha d, \quad i = 1, \ldots, n-1. \tag{5}$$

Then, by Corollary 2.5 and the left inequality of (5), we have $\partial_i(G-v) + \alpha \leq \partial_i(G)$, for $i = 1, \ldots, n-1$. Similarly, by Corollary 2.5 and the right inequality of (5), we get $\partial_{i+1}(G) \leq \partial_i(G-v) + \alpha d$, for $i = 1, \ldots, n-1$. □

Corollary 4.2. *Let G be a graph of order n and with diameter $d = 2$. Suppose vertex v is adjacent to any other vertex of G. Also $G-v$ is connected with $d(G-v) = d(G)$; then $\partial_{i+1}(G) - \alpha \leq \partial_i(G-v) \leq \partial_i(G) - \alpha$, for $i = 1, 2, \ldots, n-1$.*

Proof. Using the given assumptions, we obtain $d_{G-v}(x,y) = d_G(x,y)$ for $x, y \in V(G-v)$, hence $Tr_G(z) = Tr_{G-v}(z) + 1$. Let M be the principal submatrix of $D_\alpha(G)$ obtained by deleting the row and column corresponding to v and $S = M - D_\alpha(G-v) = \alpha I$. By Lemma 2.4, we get $\partial_i(G-v) + \alpha \leq \lambda_i(M) \leq \partial_i(G-v) + \alpha$, $i = 1, \ldots, n-1$. Hence, similarly to Theorem 4.1, we get the desired result. □

Corollary 4.3. *Let G be a graph of order n and $u, v \in V(G)$. If u, v are multiplicate (or quasimultiplicate) vertices, then $\partial_{i+1}(G) - \alpha d \leq \partial_i(G-v) \leq \partial_i(G) - \alpha$, for $i = 1, 2, \ldots, n-1$.*

The following lemma is on the behaviour of generalized distance eigenvalues when the edge between quasi-multiplicate vertices is removed.

Lemma 4.4. *Let G be a graph of order $n \geq 3$. Also, let x and y be quasi-multiplicate vertices of G and $e = xy$. Then, we have*
(i) if $\alpha \geq \frac{1}{2}$, then $\partial_i(G) \leq \partial_i(G-e) \leq \partial_i(G) + 1$,
(ii) if $\alpha < \frac{1}{2}$, then $\partial_i(G) + 2\alpha - 1 \leq \partial_i(G-e) \leq \partial_i(G) + 1$, for $i = 1, 2, \ldots, n$.

Proof. Since x and y are quasi-multiplicate vertices, apart from the change of $d(x,y) = 1$ to $d(x,y) = 2$, the distances of other vertices are fixed. So $D_\alpha(G-e) > D_\alpha(G)$. Let $S = D_\alpha(G-e) - D_\alpha(G)$. Then S can be partitioned into $S = \begin{pmatrix} \alpha I + (1-\alpha)(J_2 - I) & 0 \\ 0 & 0 \end{pmatrix}$.
Hence the eigenvalues of S are $\{1, 2\alpha - 1, 0^{[n-2]}\}$. Thus, the conclusion follows by Lemma 2.4. □

The following gives the behaviour of generalized distance eigenvalues when the edges between the vertices in a quasi-multiplicate set are deleted.

THEOREM 4.5. *Let $U \subset V(G)$ be a quasi-multiplicate set of graph G and $2 \leq m = |U| < n = |V(G)|$. Suppose G^c is the graph obtained by removing all the edges between vertices of U. Then we have*
(i) if $\alpha \geq \frac{1}{m}$, then $\partial_i(G) \leq \partial_i(G^c) \leq \partial_i(G) + m - 1$,

(ii) if $\alpha < \frac{1}{m}$, then $\partial_i(G) + \alpha m - 1 \leq \partial_i(G^c) \leq \partial_i(G) + m - 1$, for $i = 1, 2, \ldots, n$.

Proof. Obviously, U becomes a multiplicate set in G^c. Similar to Lemma 4.4, in the process of deleting edges, only the distances of vertices in U change from one to two. Let $S = D_\alpha(G^c) - D_\alpha(G)$. Then S can be partitioned into $S = \begin{pmatrix} R & 0 \\ 0 & 0 \end{pmatrix}$, where $R = \alpha(m-1)I + (1-\alpha)(J_m - I)$. Hence the eigenvalues of R are $\{m-1, \alpha m - 1^{[m-1]}\}$. Then the eigenvalues of S are $\{m - 1, \alpha m - 1^{[m-1]}, 0^{[n-m]}\}$. Thus, the result follows from Lemma 2.4. $\square$

The following result gives the graph with the minimum $\partial(G)$ among all the trees with given diameter d.

THEOREM 4.6. *Let Υ_d be the set of all trees with diameter $d \geq 1$, and $\alpha > 0$. Also, let P_{d+1} denotes the path of order $d+1$. Then for any tree $T \in \Upsilon_d$, we have $\partial(T) \geq \partial(P_{d+1})$. Equality occurs if and only if $T = P_{d+1}$.*

Proof. Let T be a tree of order n. Suppose that $T \in \Upsilon_d$ with order $n \geq d + 1$. From Theorem 4.1, we see that $\partial(G - u) \leq \partial(G) - \alpha$, where u is a pendent vertex. Hence, the generalized distance spectral radius $\partial(G)$ strictly decreases for $\alpha > 0$, when the pendent vertices are removed from G. Then, the result follows by continuously deleting the pendent vertices which are not on the diametrical line. $\square$

Recall that the *girth* of a graph G is the length of the shortest cycle in G. The following result gives the graph with the minimum $\partial(G)$ among all the unicyclic graphs with given girth.

THEOREM 4.7. *Let Γ_p be the set of all unicyclic graphs of order n with given girth $p \geq 3$. For any unicyclic graph $G \in \Gamma_p$, we have*

$$\partial(G) \geq \begin{cases} \frac{p^2}{4} & \text{if } p \text{ is even} \\ \frac{p^2-1}{4} & \text{if } p \text{ is odd,} \end{cases}$$

with equality if and only if $G = C_p$.

Proof. Let G be a connected graph of order n. Suppose that $G \in \Gamma_p$; then girth of G is p and so G contains a cycle of length p. Let us partition the vertex set of G as $V(G) = A_1 \cup A_2$, where the vertex set of the cycle is $A_1 = \{a_1, \ldots, a_p\}$. Then the components of subgraph induced by $A_2 = \{a_{p+1}, \ldots, a_n\}$ are isolated vertices or trees. Assume that G has the minimum generalized distance spectral radius with order $n > p$, then $A_2 \neq \varnothing$. By Theorem 4.1, we obtain another graph $G - a_i$

with less generalized distance spectral radius, where $a_i \in A_2$ is a pendent vertex, a contradiction. Thus $G = C_p$ has the minimum generalized distance spectral radius. It is well known that

$$W(C_n) = \begin{cases} \frac{n^3}{8} & \text{if } n \text{ is even} \\ \frac{n(n^2-1)}{8} & \text{if } n \text{ is odd.} \end{cases}$$

The result now follows from Lemma 2.1. □

5. The generalized distance spectrum of some graphs

Recall that the k-th power G^k of a graph G is a graph with the same set of vertices $V(G)$ and two vertices are adjacent when their distance in G is at most k. In this section, we obtain the generalized distance spectrum of the square of the cycle and the square of the hypercube of dimension n. We show that the square of the hypercube of dimension n has three distinct generalized distance eigenvalues.

The following lemma can be found in [16].

Lemma 5.1 ([16]). *Let*

$$A = \begin{pmatrix} A_0 & A_1 \\ A_1 & A_0 \end{pmatrix}$$

be a 2×2 block symmetric matrix. Then the eigenvalues of A are those of $A_0 + A_1$ together with those of $A_0 - A_1$.

The following gives the generalized distance spectrum of the square of the cycle.

Theorem 5.2. *Let $\{\frac{n^2}{4}, 0, \lambda_3, \ldots, \lambda_n\}$ or $\{\frac{n^2}{4}, -1, \lambda_3, \ldots, \lambda_n\}$ be the distance spectrum of C_n depending on whether $\frac{n}{2}$ is even or odd. Then generalized distance spectrum of C_n^2 is given by*

$$\left\{\frac{n^2+2n}{8}, \alpha\left(\frac{n^2+4n}{8}\right) - \frac{n}{4}, \alpha\left(\frac{n^2+2n-4\lambda_3}{8}\right) + \frac{\lambda_3}{2}, \ldots, \alpha\left(\frac{n^2+2n-4\lambda_n}{8}\right) + \frac{\lambda_n}{2}\right\},$$

where $\frac{n}{2}$ is even, and

$$\left\{\frac{n^2+2n}{8}, \alpha\left(\frac{(n+2)^2}{8}\right) - \frac{n+2}{4}, \alpha\left(\frac{n^2+2n-4\lambda_3}{8}\right) + \frac{\lambda_3}{2}, \ldots, \alpha\left(\frac{n^2+2n-4\lambda_n}{8}\right) + \frac{\lambda_n}{2}\right\},$$

where $\frac{n}{2}$ is odd.

Proof. Let $\{u_1, u_2, \ldots, u_n\}$ be the vertex set of C_n. Let us partition the vertex set of C_n as $V_1 \cup V_2$ where V_1 is a set of all even index vertices and V_2 is a set of all odd index vertices. Then every pair of vertices within V_1 or within V_2 are of even distance from each other. Again any vertex of V_1 and any vertex of V_2 are of odd distance from each other. Now, if we index the rows and columns of the generalized distance matrix by taking the vertices of V_1 followed by the vertices of V_2 and by considering a suitable ordering, we get the generalized distance matrix of C_n in the form

$$D_\alpha(C_n) = \begin{pmatrix} \alpha K + (1-\alpha)S & (1-\alpha)U \\ (1-\alpha)U & \alpha K + (1-\alpha)S \end{pmatrix},$$

where each entry of the block S is even and any row in S is equal to the sum of the distances from any vertex in V_1 to all other vertices in V_1, hence S has constant row sum $r(S)$. Again, each entry of the block U is even and any row in U is equal to the sum of the distances from any vertex in V_1 to all other vertices in V_2, hence U has constant row sum $r(U)$, which is

$$r(S) = \begin{cases} \frac{n^2-4}{8} & \text{if } \frac{n}{2} \text{ is odd} \\ \frac{n^2}{8} & \text{if } \frac{n}{2} \text{ is even} \end{cases}, \quad r(U) = \begin{cases} \frac{n^2+4}{8} & \text{if } \frac{n}{2} \text{ is odd} \\ \frac{n^2}{8} & \text{if } \frac{n}{2} \text{ is even.} \end{cases}$$

Also $K = \left(\frac{n^2}{4}\right) I$. Therefore the generalized distance matrix of C_n^2 has the form

$$D_\alpha(C_n^2) = \frac{1}{2}\begin{pmatrix} \alpha P + (1-\alpha)S & (1-\alpha)(U + J_{\frac{n}{2}\times\frac{n}{2}}) \\ (1-\alpha)(U + J_{\frac{n}{2}\times\frac{n}{2}}) & \alpha P + (1-\alpha)S \end{pmatrix},$$

where $P = \left(\frac{n^2+2n}{4}\right) I$. Now, using Lemma 5.1, the eigenvalues of $D_\alpha(C_n^2)$ are the union of the eigenvalues of $\frac{1}{2}(\alpha P + (1-\alpha)(S+U+J))$ and $\frac{1}{2}(\alpha P + (1-\alpha)(S-U-J))$. Hence, if $\frac{n}{2}$ is even, then

$$\begin{aligned} spec(D_\alpha(C_n^2)) = \Big\{ &\alpha\left(\frac{n^2+2n}{8}\right) + (1-\alpha)\left(\frac{n^2}{8}+\frac{n}{4}\right), \alpha\left(\frac{n^2+2n}{8}\right) - (1-\alpha)\left(\frac{n}{4}\right), \\ &\alpha\left(\frac{n^2+2n}{8}\right) + (1-\alpha)\left(\frac{\lambda_3}{2}\right), \dots, \alpha\left(\frac{n^2+2n}{8}\right) + (1-\alpha)\left(\frac{\lambda_n}{2}\right)\Big\}, \end{aligned}$$

and if $\frac{n}{2}$ is odd, then

$$\begin{aligned} spec(D_\alpha(C_n^2)) = \Big\{ &\alpha\left(\frac{n^2+2n}{8}\right) + (1-\alpha)\left(\frac{n^2}{8}+\frac{n}{4}\right), \alpha\left(\frac{n^2+2n}{8}\right) - (1-\alpha)\left(\frac{1}{2}+\frac{n}{4}\right), \\ &\alpha\left(\frac{n^2+2n}{8}\right) + (1-\alpha)\left(\frac{\lambda_3}{2}\right), \dots, \alpha\left(\frac{n^2+2n}{8}\right) + (1-\alpha)\left(\frac{\lambda_n}{2}\right)\Big\}. \end{aligned}$$

Therefore, we get the desired result. □

The *Hamming graph* $H(n,d)$ has vertex set X^n where X is a finite set of cardinality $d \geq 2$, and two vertices of $H(n,d)$ are adjacent whenever they differ in precisely one coordinate. In particular, the n-dimensional hypercube Q_n is $H(n,2)$.

LEMMA 5.3 ([20]). *Let $H(n,d)$ be the Hamming graph of diameter n. Then the distance spectrum of $H(n,d)$ is* $\left\{nd^{n-1}(d-1)^{[1]}, 0^{[d^n-n(d-1)-1]}, (-d^{n-1})^{[n(d-1)]}\right\}$.

We recall that an *n-dimensional hypercube* Q_n is a graph with vertex set $V(Q_n) = \{(a_1, a_2, \dots, a_n) : a_i = 0 \text{ or } 1\}$ and two vertices of Q_n are adjacent if and only if they differ at exactly one coordinate. For $u, v \in V(Q_n)$, it is clear that $d(u,v) = r$ if and only if coordinates of u and v differ in exactly r places.

The following gives the generalized distance spectrum of the square of the hypercube of dimension n.

THEOREM 5.4. *Let Q_n be the hypercube graph of dimension n. Then the generalized distance spectrum of Q_n^2 is*

$$\left\{ (\frac{1}{2}\sum_{i=1}^{n} i\binom{n}{i} + 2^{n-2})^{[1]}, \right.$$
$$\left. \alpha\left(\frac{1}{2}\sum_{i=1}^{n} i\binom{n}{i} + 2^{n-2}\right)^{[2^n-(n+2)]}, (\alpha\left(\frac{1}{2}\sum_{i=1}^{n} i\binom{n}{i} + 2^{n-1}\right) - 2^{n-2})^{[n+1]} \right\}.$$

Proof. Consider the vertex $x = (0, 0, \ldots, 0)$. Let V_1 be the set of vertices of Q_n which are of even distance from x and let V_2 be the set of vertices of Q_n which are of odd distance from x. All vertices within V_1 and those within V_2 are of even distance from each other. Again any vertex of V_1 and any vertex of V_2 are of odd distance from each other. Considering a suitable ordering of the vertices of V_1 and V_2, the generalized distance matrix of Q_n is of the form

$$D_\alpha(Q_n) = \begin{pmatrix} \alpha K + (1-\alpha)S & (1-\alpha)U \\ (1-\alpha)U & \alpha K + (1-\alpha)S \end{pmatrix},$$

where U and S have same properties as in the Theorem 5.2 and $K = \left(\sum_{i=1}^{n} i\binom{n}{i}\right) I$, since the sum of the distances from any vertex in V_1 to all other vertices in V_1 is given by

$$k_1 = \begin{cases} \sum_i i\binom{n}{i}, & i \in 2k,\ k = 1, 2, \ldots, \frac{n-1}{2} \quad \text{if } n \text{ is odd} \\ \sum_i i\binom{n}{i}, & i \in 2k,\ k = 1, 2, \ldots, \frac{n}{2} \quad \text{if } n \text{ is even.} \end{cases}$$

Again, the sum of the distances from any vertex in V_1 to all vertices in V_2 is given by

$$k_2 = \begin{cases} \sum_i i\binom{n}{i}, & i \in 2k-1,\ k = 1, 2, \ldots, \frac{n+1}{2} \quad \text{if } n \text{ is odd} \\ \sum_i i\binom{n}{i}, & i \in 2k-1,\ k = 1, 2, \ldots, \frac{n}{2} \quad \text{if } n \text{ is even.} \end{cases}$$

Hence for each n, the matrix $U+S$ has constant row sum $k_1+k_2 = \sum_{i=1}^{n} i\binom{n}{i}$ and the matrix $U-S$ has constant row sum $k_1 - k_2 = 0$. Therefore, the generalized distance matrix of Q_n^2 has the form

$$D_\alpha(Q_n^2) = \frac{1}{2}\begin{pmatrix} \alpha F + (1-\alpha)S & (1-\alpha)(U + J_{2^{n-1}\times 2^{n-1}}) \\ (1-\alpha)(U + J_{2^{n-1}\times 2^{n-1}}) & \alpha F + (1-\alpha)S \end{pmatrix},$$

where $F = \left(\sum_{i=1}^{n} i\binom{n}{i} + 2^{n-1}\right) I$. Now, using Lemma 5.1, the eigenvalues of $D_\alpha(Q_n^2)$ are the union of the eigenvalues of $\frac{1}{2}(\alpha F + (1-\alpha)(S + U + J_{2^{n-1}\times 2^{n-1}}))$ and $\frac{1}{2}(\alpha F + (1-\alpha)(-S - U - J_{2^{n-1}\times 2^{n-1}}))$, hence we have

$$\left\{ \alpha\left(\frac{1}{2}\sum_{i=1}^{n} i\binom{n}{i} + 2^{n-2}\right) + (1-\alpha)\left(\frac{1}{2}\sum_{i=1}^{n} i\binom{n}{i} + 2^{n-2}\right), \right.$$
$$\left. \alpha\left(\frac{1}{2}\sum_{i=1}^{n} i\binom{n}{i} + 2^{n-2}\right) + 0, \alpha\left(\frac{1}{2}\sum_{i=1}^{n} i\binom{n}{i} + 2^{n-2}\right) - (1-\alpha)2^{n-2} \right\}.$$

Then by Lemma 5.3, we get the desired result. □

It is clear from Theorem 5.4 that the graph Q_n^2 has three distinct generalized distance eigenvalues.

Acknowledgement. The research of K. C. Das is supported by National Research Foundation funded by the Korean government (Grant No. 2021R1F1A1050646).

The authors would like to thank the anonymous referee and the handling editor for their constructive comments that helped improve the quality of this paper.

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(received 25.04.2022; in revised form 20.12.2022; available online 20.06.2023)

Faculty of Mathematical Sciences, Shahrood University of Technology, Shahrood, Iran

E-mail: a.alhevaz@shahroodut.ac.ir

Faculty of Mathematical Sciences, Shahrood University of Technology, Shahrood, Iran

E-mail: maryamb8989@gmail.com

Department of School Education, JK Govt. Kashmir, India

E-mail: hilahmad1119kt@gmail.com

Department of Mathematics, Sungkyunkwan University, Suwon 16419, Republic of Korea

E-mail: kinkardas2003@gmail.com