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Sharp Bounds on (Generalized) Distance Energy of Graphs

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Abstract: Given a simple connected graph G , let $D(G)$ be the distance matrix, $D^L(G)$ be the distance Laplacian matrix, $D^Q(G)$ be the distance signless Laplacian matrix, and $Tr(G)$ be the vertex transmission diagonal matrix of G . We introduce the generalized distance matrix $D_\alpha(G) = \alpha Tr(G) + (1 - \alpha)D(G)$, where $\alpha \in [0, 1]$. Noting that $D_0(G) = D(G)$, $2D_{\frac{1}{2}}(G) = D^Q(G)$, $D_1(G) = Tr(G)$ and $D_\alpha(G) - D_\beta(G) = (\alpha - \beta)D^L(G)$, we reveal that a generalized distance matrix ideally bridges the spectral theories of the three constituent matrices. In this paper, we obtain some sharp upper and lower bounds for the generalized distance energy of a graph G involving different graph invariants. As an application of our results, we will be able to improve some of the recently given bounds in the literature for distance energy and distance signless Laplacian energy of graphs. The extremal graphs of the corresponding bounds are also characterized.

Keywords: distance energy; distance (signless) Laplacian energy; generalized distance energy; transmission regular graph.

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1. Introduction

We study in this paper simple connected graphs $G = (V, E)$ with $V(G) = \{v_1, v_2, \dots, v_n\}$ being the vertex set and $E(G)$ being the edge set. The order of G is denoted by $|V(G)| = n$ and the size of G is denoted by $|E(G)| = m$. Let $N(v)$ be the neighborhood of a vertex v in $V(G)$. Let \bar{G} represent the complement of G . Some classical graphs such as the complete graph, complete bipartite graph, path, and cycle are denoted by K_n , $K_{s,t}$, P_n , and C_n , respectively. The degree of v is denoted by $d_G(v)$ or simply d_v . The adjacency matrix is $A(G) = (a_{ij})$ with $\text{Deg}(G) = \text{diag}(d_1, d_2, \dots, d_n)$ being the diagonal degree matrix with $d_i = d_G(v_i)$, $i = 1, 2, \dots, n$. The Laplacian and signless Laplacian matrices are signified by $L(G) = \text{Deg}(G) - A(G)$ and $Q(G) = \text{Deg}(G) + A(G)$, respectively. Their spectra are arranged as $0 = \mu_n \leq \mu_{n-1} \leq \dots \leq \mu_1$ and $0 \leq q_n \leq q_{n-1} \leq \dots \leq q_1$, respectively.

Let d_{uv} be the graph distance between two vertices u and v . The distance matrix of G is given by $D(G) = (d_{uv})_{u,v \in V(G)}$. The transmission of a vertex v is $Tr_G(v) = \sum_{u \in V(G)} d_{uv}$. If $Tr_G(v) = k$, for each $v \in V(G)$, then G is called k -transmission regular. The Wiener index or transmission is defined as $W(G) = \frac{1}{2} \sum_{v \in V(G)} Tr_G(v)$. The transmission $Tr_G(v_i)$ or simply Tr_i forms a sequence $\{Tr_1, Tr_2, \dots, Tr_n\}$,

which is usually referred to as the transmission degree sequence of G . The quantity $T_i = \sum_{j=1}^n d_{ij} Tr_j$ means the second transmission degree of v_i .

Let $Tr(G) = \text{diag}(Tr_1, Tr_2, \dots, Tr_n)$ be the diagonal matrix containing vertex transmission. Aouchiche and Hansen [1–3] studied the two matrices $D^L(G) = Tr(G) - D(G)$ and $D^Q(G) = Tr(G) + D(G)$, which are referred to as the distance Laplacian matrix and distance signless Laplacian matrix, respectively. Thus far, the spectral properties of $D(G)$, $D^L(G)$ and $D^Q(G)$ of connected undirected graph G have been investigated extensively. For some recent works in this subject, see [1–15] as well as the references therein.

Recently, Cui et al. [16] considered some convex combinations of the distance matrix and the diagonal matrix with vertex transmissions of undirected graphs, which can underpin a unified theory of distance spectral theories. The *generalized distance matrix* $D_\alpha(G)$ is a convex combinations of $Tr(G)$ and $D(G)$, and defined as $D_\alpha(G) = \alpha Tr(G) + (1 - \alpha)D(G)$, for $0 \leq \alpha \leq 1$. Since $D_0(G) = D(G)$, $2D_{\frac{1}{2}}(G) = D^Q(G)$, $D_1(G) = Tr(G)$ and $D_\alpha(G) - D_\beta(G) = (\alpha - \beta)D^L(G)$, the generalized distance matrix spectral theory ideally encompasses those for distance matrix and distance (signless) Laplacian matrices. The eigenvalues of $D_\alpha(G)$ can be ordered as $\partial_1 \geq \partial_2 \geq \dots \geq \partial_n$. We will denote by $\text{spec}(G)$ the generalized distance spectrum of the graph G . For some recent works on the generalized distance spectrum, we direct readers to consult the papers [8,16–20].

The energy of a graph [21] as a mathematical chemistry concept was put forward by Ivan Gutman. In chemistry, the energy is used to approximate the total Π -electron energy of a molecule. Let $\lambda_1, \lambda_2, \dots, \lambda_n$ be the adjacency eigenvalues of a graph G . The *energy* of a graph G , denoted by $E(G)$, is defined as $E(G) = \sum_{i=1}^n |\lambda_i|$ (see [22] for an updated survey). Recently, other kinds of energies of a graph have been defined and studied. We recall some of them. Let $\rho_1^D \geq \rho_2^D \geq \dots \geq \rho_n^D$ and $\rho_1^L \geq \rho_2^L \geq \dots \geq \rho_n^L$ and also $\rho_1^Q \geq \rho_2^Q \geq \dots \geq \rho_n^Q$ represent the distance, distance Laplacian, and distance signless Laplacian eigenvalues, respectively. The distance energy of a graph G was introduced in [23] as

$$E^D(G) = \sum_{i=1}^n |\rho_i^D|.$$

We have

$$\sum_{i=1}^n \rho_i^D = 0 \text{ and } \sum_{i=1}^n (\rho_i^D)^2 = 2 \sum_{1 \leq i < j \leq n} (d_{ij})^2. \quad (1)$$

For some recent results on the distance energy of a graph, we refer to [10] and the references therein.

In addition, the concept of distance Laplacian and distance signless Laplacian energies were introduced in [7,10,24], respectively, as follows. The distance Laplacian energy of a graph G is defined by taking into consideration of distance Laplacian spectrum deviations as

$$E^L(G) = \sum_{i=1}^n \left| \rho_i^L - \frac{2W(G)}{n} \right|.$$

Similarly, the distance signless Laplacian energy of a graph G is defined as follows:

$$E^Q(G) = \sum_{i=1}^n \left| \rho_i^Q - \frac{2W(G)}{n} \right|.$$

For some recent papers on $E^L(G)$ and $E^Q(G)$, we refer to [7,10,25], and for other recent papers regarding the energy of a matrix with respect to different graph matrices; see [11,12,23,26–29] and the references therein.

Motivated by the definitions of $E^L(G)$ and $E^Q(G)$, Alhevaz et al. [17] recently defined the generalized distance energy of G as the average deviation of generalized distance spectrum:

$$E^{D_\alpha}(G) = \sum_{i=1}^n |\Theta_i|,$$

where

$$\Theta_i = \partial_i - \frac{2\alpha W(G)}{n}.$$

As $\sum_{i=1}^n \partial_i = 2\alpha W(G)$ and $\sum_{i=1}^n \partial_i^2 = \text{trace}[D_\alpha(G)]^2 = 2(1-\alpha)^2 \sum_{1 \leq i < j \leq n} (d_{ij})^2 + \alpha^2 \sum_{i=1}^n Tr_i^2$, hence by the definition of Θ_i , one can easily see that $\sum_{i=1}^n \Theta_i = 0$ and $\sum_{i=1}^n \Theta_i^2 = P$, where

$$P = 2(1-\alpha)^2 \sum_{1 \leq i < j \leq n} (d_{ij})^2 + \alpha^2 \sum_{i=1}^n Tr_i^2 - \frac{4\alpha^2 W^2(G)}{n}.$$

From the above definition, $E^{D_0}(G) = E^D(G)$ and $2E^{D_{\frac{1}{2}}}(G) = E^Q(G)$. Thus, exploring the properties of $E^{D_\alpha}(G)$ and its dependency with parameter α could give us a unified picture of the spectral properties of distance (signless Laplacian) energy of graphs.

The rest of the paper is structured as follows. In Section 2, for $\alpha \in [0, 1]$, we obtain some sharp lower bounds for the generalized distance energy $E^{D_\alpha}(G)$ of a connected graph G resorting to Wiener index $W(G)$, transmission degrees, and the parameter $\alpha \in [0, 1]$. The graphs attaining the corresponding bounds are also characterized. In Section 3, we obtain sharp upper bounds for the generalized distance energy $E^{D_\alpha}(G)$ involving diameter d , minimum degree δ , Wiener index $W(G)$, as well as transmission degrees. Some extremal graphs that attain these bounds are determined in this section. As an application of our results in Section 3, we will be able to improve some recently given upper bounds for distance (signless Laplacian) energy in [25].

2. Lower Bounds for $E^{D_\alpha}(G)$

In this section, we give some sharp lower bounds for $E^{D_\alpha}(G)$ in terms of different graph parameters. Firstly, we include some previous known results that will play a pivotal role in the rest of the paper.

Lemma 1 ([16]). *If G is a connected graph, then*

$$\partial(G) \geq \frac{2W(G)}{n},$$

where the equality holds if and only if G is transmission regular.

Lemma 2. *Recall that $\{Tr_1, Tr_2, \dots, Tr_n\}$ constitutes the transmission degrees. We have*

$$\partial(G) \geq \sqrt{\frac{\sum_{i=1}^n Tr_i^2}{n}},$$

where the equality holds if and only if G is transmission regular.

Proof. This lemma follows from (Theorem 2.2 [7]). \square

Lemma 3 ([16]). Recall the second transmission degree sequence of G is $\{T_1, T_2, \dots, T_n\}$. We have

$$\partial(G) \geq \sqrt{\frac{\sum_{i=1}^n (\alpha Tr_i^2 + (1-\alpha)T_i)^2}{\sum_{i=1}^n Tr_i^2}}.$$

Moreover, if $\frac{1}{2} \leq \alpha \leq 1$, the equality holds if and only if G is transmission regular.

Remark 1. Keeping all of the notations from Lemma 3, we have

$$\partial(G) \geq \sqrt{\frac{\sum_{i=1}^n (\alpha Tr_i^2 + (1-\alpha)T_i)^2}{\sum_{i=1}^n Tr_i^2}} \geq \frac{2W(G)}{n}.$$

In fact, as we always have $\sum_{i=1}^n T_i = \sum_{i=1}^n Tr_i^2$, and also applying the Cauchy–Schwarz inequality, we have $(\sum_{i=1}^n T_i)^2 \leq n \sum_{i=1}^n T_i^2$ and $(\sum_{i=1}^n Tr_i)^2 \leq n \sum_{i=1}^n Tr_i^2$. Hence, we get

$$\begin{aligned} \partial(G) &\geq \sqrt{\frac{\sum_{i=1}^n (\alpha Tr_i^2 + (1-\alpha)T_i)^2}{\sum_{i=1}^n Tr_i^2}} \\ &\geq \sqrt{\frac{(\sum_{i=1}^n (\alpha Tr_i^2 + (1-\alpha)T_i))^2}{n \sum_{i=1}^n Tr_i^2}} \\ &= \sqrt{\frac{(\sum_{i=1}^n Tr_i^2)^2}{n \sum_{i=1}^n Tr_i^2}} = \sqrt{\frac{\sum_{i=1}^n Tr_i^2}{n}} \geq \sqrt{\frac{(\sum_{i=1}^n Tr_i)^2}{n^2}} = \frac{2W(G)}{n}. \end{aligned}$$

Lemma 4 ([30]). Assume that a_i and b_i , $i = 1, 2, \dots, n$, are positive real numbers. We have

$$\sum_{i=1}^n a_i^2 \sum_{i=1}^n b_i^2 \leq \frac{1}{4} \left(\sqrt{\frac{M_1 M_2}{m_1 m_2}} + \sqrt{\frac{m_1 m_2}{M_1 M_2}} \right)^2 \left(\sum_{i=1}^n a_i b_i \right)^2, \quad (2)$$

where $M_1 = \max_{1 \leq i \leq n} a_i$, $M_2 = \max_{1 \leq i \leq n} b_i$, $m_1 = \min_{1 \leq i \leq n} a_i$ and $m_2 = \min_{1 \leq i \leq n} b_i$.

Lemma 5 ([31]). If b_1, b_2, \dots, b_n are positive numbers, then:

$$\frac{a_1 + a_2 + \dots + a_n}{b_1 + b_2 + \dots + b_n} \leq \max_{1 \leq i \leq n} \frac{a_i}{b_i},$$

for any real numbers a_1, a_2, \dots, a_n . Equality holds if and only if $\frac{a_i}{b_i}$ are equal for all i .

The following lemma characterizes the graphs with exactly two distinct generalized distance eigenvalues.

Lemma 6. A connected graph G possesses precisely two different $D_\alpha(G)$ eigenvalues if and only if it is a complete graph.

Proof. The proof is analogous to that of (Lemma 2.10 [32]). \square

Our first lower bound for the generalized distance energy $E^{D_\alpha}(G)$ relies on the Wiener index $W(G)$ as well as the transmission degrees.

Theorem 1. Assume that G is a connected graph with $n > 1$ nodes. We have

$$E^{D_\alpha}(G) \geq n \left| \det \left(D_\alpha(G) - \frac{2\alpha W(G)}{n} \right) \right|^{\frac{1}{n}},$$

where the equality holds if and only if G is a complete graph.

Proof. By the Cauchy–Schwarz inequality, we have

$$\sum_{i=1}^n \sqrt{\left| \partial_i - \frac{2\alpha W(G)}{n} \right|} \leq \sqrt{n \left(\sum_{i=1}^n \left| \partial_i - \frac{2\alpha W(G)}{n} \right| \right)}, \quad (3)$$

that is,

$$\sqrt{E^{D_\alpha}(G)} \geq \frac{\sum_{i=1}^n \sqrt{\left| \partial_i - \frac{2\alpha W(G)}{n} \right|}}{\sqrt{n}}.$$

Since

$$\begin{aligned} & \frac{\sqrt{\left| \partial_1 - \frac{2\alpha W(G)}{n} \right|} + \sqrt{\left| \partial_2 - \frac{2\alpha W(G)}{n} \right|} + \dots + \sqrt{\left| \partial_n - \frac{2\alpha W(G)}{n} \right|}}{n} \\ & \geq \left(\sqrt{\left| \partial_1 - \frac{2\alpha W(G)}{n} \right|} \left| \partial_2 - \frac{2\alpha W(G)}{n} \right| \dots \left| \partial_n - \frac{2\alpha W(G)}{n} \right| \right)^{\frac{1}{n}}, \end{aligned}$$

hence we get

$$\sqrt{E^{D_\alpha}(G)} \geq \sqrt{n} \left(\sqrt{\left| \partial_1 - \frac{2\alpha W(G)}{n} \right|} \left| \partial_2 - \frac{2\alpha W(G)}{n} \right| \dots \left| \partial_n - \frac{2\alpha W(G)}{n} \right| \right)^{\frac{1}{n}}.$$

Thus, we have $E^{D_\alpha}(G) \geq n \left| \det \left(D_\alpha(G) - \frac{2\alpha W(G)}{n} \right) \right|^{\frac{1}{n}}$.

Suppose that equality holds. Then, from equality in (3), we get

$$\sqrt{\left| \partial_1 - \frac{2\alpha W(G)}{n} \right|} = \sqrt{\left| \partial_2 - \frac{2\alpha W(G)}{n} \right|} = \dots = \sqrt{\left| \partial_n - \frac{2\alpha W(G)}{n} \right|}.$$

Hence, G has exactly one distinct D_α -eigenvalue or G has exactly two distinct D_α -eigenvalues. In view of Lemma 6, we get $G \cong K_n$, and the proof is complete. \square

Next, we give a lower bound for $E^{D_\alpha}(G)$ utilizing only the Wiener index $W(G)$.

Theorem 2. Assume that G is a connected graph having n vertices. Suppose that $\alpha \leq 1 - \frac{n}{2W(G)}$. Then,

$$E^{D_\alpha}(G) \geq (1 - \alpha) \frac{2W(G)}{n} + n - 1 + \ln \Delta - \ln \left((1 - \alpha) \frac{2W(G)}{n} \right), \quad (4)$$

where $\Delta = \left| \det \left(D_\alpha(G) - \frac{2\alpha W(G)}{n} I \right) \right|$. The equality in (4) holds if and only if $\alpha = 0$ and $G \cong K_n$ or G is a k -transmission regular graph with three different generalized distance eigenvalues represented as $k, \alpha k + 1$ and $\alpha k - 1$.

Proof. We construct a function

$$f(x) = x - \frac{2\alpha W(G)}{n} - 1 - \ln \left(x - \frac{2\alpha W(G)}{n} \right)$$

for $x - \frac{2\alpha W(G)}{n} > 0$. It is elementary to prove that $f(x)$ is increasing for $x - \frac{2\alpha W(G)}{n} \geq 1$ and decreasing for $0 < x - \frac{2\alpha W(G)}{n} \leq 1$. Consequently, $f(x) \geq f\left(\frac{2\alpha W(G)}{n} + 1\right) = 0$, implying that $x - \frac{2\alpha W(G)}{n} \geq 1 + \ln\left(x - \frac{2\alpha W(G)}{n}\right)$ for $x - \frac{2\alpha W(G)}{n} > 0$, with equality holding if and only if $x - \frac{2\alpha W(G)}{n} = 1$. With these at hand, we get

$$\begin{aligned} E^{D_\alpha}(G) &= \partial_1 - \frac{2\alpha W(G)}{n} + \sum_{i=2}^n \left| \partial_i - \frac{2\alpha W(G)}{n} \right| \\ &\geq \partial_1 - \frac{2\alpha W(G)}{n} + n - 1 + \sum_{i=2}^n \ln \left| \partial_i - \frac{2\alpha W(G)}{n} \right| \end{aligned} \quad (5)$$

$$\begin{aligned} &= \partial_1 - \frac{2\alpha W(G)}{n} + n - 1 + \ln \prod_{i=2}^n \left| \partial_i - \frac{2\alpha W(G)}{n} \right| \\ &= \partial_1 - \frac{2\alpha W(G)}{n} + n - 1 + \ln \Delta - \ln \left(\partial_1 - \frac{2\alpha W(G)}{n} \right). \end{aligned} \quad (6)$$

From Lemma 1, we know that $\partial_1 \geq \frac{2W(G)}{n}$. Consider the function

$$g(x) = x - \frac{2\alpha W(G)}{n} + n - 1 + \ln \Delta - \ln \left(x - \frac{2\alpha W(G)}{n} \right).$$

It is straightforward to see that $g(x)$ is an increasing function on $1 \leq x - \frac{2\alpha W(G)}{n} \leq n$. Since for $\alpha \leq 1 - \frac{n}{2W(G)}$ we have $x - \frac{2\alpha W(G)}{n} \geq (1 - \alpha) \frac{2W(G)}{n} \geq 1$, it follows that

$$g(x) \geq g\left(\frac{2W(G)}{n}\right) = (1 - \alpha) \frac{2W(G)}{n} + n - 1 + \ln \Delta - \ln \left((1 - \alpha) \frac{2W(G)}{n} \right).$$

In the light of these results and (5), we derive (4).

Suppose the equality holds in (4). Then, $\partial_1 = \frac{2W(G)}{n}$ and so, by Lemma 1, G is a transmission regular graph. From equality in (5), we get $\left| \partial_i - \frac{2\alpha W(G)}{n} \right| = 1$, for $i = 2, 3, \dots, n$. This gives that $\left| \partial_i - \frac{2\alpha W(G)}{n} \right|$ can have no more than two different values and we obtain the following:

- (i) If $\partial_i - \frac{2\alpha W(G)}{n} = 1$, for all $i = 2, 3, \dots, n$. Thus, $\partial_i = 1 + \frac{2\alpha W(G)}{n}$ for $i = 2, 3, \dots, n$, yielding that G has a pair of different generalized distance eigenvalues, $\partial_1 = \frac{2W(G)}{n}$ and $\partial_i = 1 + \frac{2\alpha W(G)}{n}$. Thus, by Lemma 6, G is complete. As the generalized distance eigenvalues of K_n are $\text{spec}(K_n) = \{n - 1, \alpha n - 1^{[n-1]}\}$, the equality cannot hold.
- (ii) If $\partial_i - \frac{2\alpha W(G)}{n} = -1$ for $i = 2, 3, \dots, n$. In this case, $\partial_i = \frac{2\alpha W(G)}{n} - 1$ for $i = 2, 3, \dots, n$. This means G has a pair of different generalized distance eigenvalues, $\partial_1 = \frac{2W(G)}{n}$ and $\partial_i = \frac{2\alpha W(G)}{n} - 1$. Thus, by Lemma 6, G is complete, which is true for $\alpha = 0$, giving that equality occurs in this case for $\alpha = 0$ and if and only if $G \cong K_n$.
- (iii) In this case, let, for some t , $\partial_i - \frac{2\alpha W(G)}{n} = 1$, for $i = 2, 3, \dots, t$ and $\partial_i - \frac{2\alpha W(G)}{n} = -1$, for $i = t + 1, \dots, n$. This indicates that G is transmission regular graph possessing three different generalized eigenvalues, $\text{spec}(G) = \left\{ \partial_1, \alpha \partial_1 + 1^{[t-1]}, \alpha \partial_1 - 1^{[n-t]} \right\}$.

On the other hand, suppose that $G \cong K_n$. Noting the generalized distance eigenvalues of K_n are $\text{spec}(K_n) = \{n - 1, \alpha n - 1^{[n-1]}\}$, and $\frac{2\alpha W(K_n)}{n} = \alpha(n - 1)$, we obtain that the equality holds in (4). In addition, if G is k -transmission regular graph possessing three different generalized distance eigenvalues $k, \alpha k + 1$ and $\alpha k - 1$, then the equality is true. \square

Now, by Remark 1 and proceeding similarly to Theorem 2, we obtain the following lower bound for $E^{D_\alpha}(G)$ using the transmission degrees as well as the second transmission degrees.

Theorem 3. Let G be a connected graph with n vertices and $\alpha \leq 1 - \frac{n}{2W(G)}$. Then,

$$E^{D_\alpha}(G) \geq \sqrt{\frac{\sum_{i=1}^n (\alpha Tr_i^2 + (1-\alpha)T_i)^2}{\sum_{i=1}^n Tr_i^2} - \frac{2\alpha W(G)}{n}} + n - 1 + \ln \Delta - \ln \left(\sqrt{\frac{\sum_{i=1}^n (\alpha Tr_i^2 + (1-\alpha)T_i)^2}{\sum_{i=1}^n Tr_i^2} - \frac{2\alpha W(G)}{n}} \right), \quad (7)$$

where $\Delta = \left| \det \left(D_\alpha(G) - \frac{2\alpha W(G)}{n} I \right) \right|$. The equality in (7) holds if and only if $\alpha = 0$ and $G \cong K_n$ or G is a k -transmission regular graph with three different generalized distance eigenvalues, namely $k, \alpha k + 1$ and $\alpha k - 1$.

We conclude this section by giving another sharp lower bound on the generalized distance energy.

Theorem 4. Let G be connected with n vertices and $\rho_n \geq (2\alpha - 1) \frac{2W(G)}{n}, \alpha \neq 1$. Then,

$$E^{D_\alpha}(G) \geq \varphi + (n-1) \left(\frac{\left| \det \left(D_\alpha(G) - \frac{2\alpha W(G)}{n} I \right) \right|}{\varphi} \right)^{\frac{1}{n-1}}, \quad (8)$$

where $\varphi = \max \left\{ \partial_1 - \frac{2\alpha W(G)}{n}, \frac{2\alpha W(G)}{n} - \partial_n \right\}$. Equality holds if and only if either G is a complete graph or a graph with exactly three distinct D_α -eigenvalues.

Proof. Applying the Cauchy–Schwarz inequality, we obtain

$$\sum_{i=2}^n \sqrt{\left| \partial_i - \frac{2\alpha W(G)}{n} \right|} \leq \sqrt{(n-1) \left(\sum_{i=2}^n \left| \partial_i - \frac{2\alpha W(G)}{n} \right| \right)}, \quad (9)$$

that is,

$$\sum_{i=2}^n \sqrt{\left| \partial_i - \frac{2\alpha W(G)}{n} \right|} \leq \sqrt{(n-1) \left(E^{D_\alpha}(G) - \left(\partial_1 - \frac{2\alpha W(G)}{n} \right) \right)}.$$

Since

$$\frac{\sqrt{\left| \partial_2 - \frac{2\alpha W(G)}{n} \right|} + \dots + \sqrt{\left| \partial_n - \frac{2\alpha W(G)}{n} \right|}}{n-1} \geq \left(\sqrt{\left| \partial_2 - \frac{2\alpha W(G)}{n} \right|} \dots \left| \partial_n - \frac{2\alpha W(G)}{n} \right| \right)^{\frac{1}{n-1}},$$

we obtain

$$\begin{aligned} \sqrt{E^{D_\alpha}(G) - \left(\partial_1 - \frac{2\alpha W(G)}{n} \right)} &\geq \frac{\sum_{i=2}^n \sqrt{\left| \partial_i - \frac{2\alpha W(G)}{n} \right|}}{\sqrt{n-1}} \\ &\geq \frac{(n-1) \left(\sqrt{\left| \partial_2 - \frac{2\alpha W(G)}{n} \right|} \left| \partial_3 - \frac{2\alpha W(G)}{n} \right| \dots \left| \partial_n - \frac{2\alpha W(G)}{n} \right| \right)^{\frac{1}{n-1}}}{\sqrt{n-1}}. \end{aligned}$$

Thus, we have

$$\begin{aligned} E^{D_\alpha}(G) &\geq \partial_1 - \frac{2\alpha W(G)}{n} + (n-1) \left(\left| \partial_2 - \frac{2\alpha W(G)}{n} \right| \left| \partial_3 - \frac{2\alpha W(G)}{n} \right| \dots \left| \partial_n - \frac{2\alpha W(G)}{n} \right| \right)^{\frac{1}{n-1}} \\ &= \partial_1 - \frac{2\alpha W(G)}{n} + (n-1) \left(\frac{\left| \det \left(D_\alpha(G) - \frac{2\alpha W(G)}{n} \right) \right|}{\partial_1 - \frac{2\alpha W(G)}{n}} \right)^{\frac{1}{n-1}}. \end{aligned}$$

Let us consider a function

$$f(x) = x + (n-1) \left(\frac{\left| \det \left(D_\alpha(G) - \frac{2\alpha W(G)}{n} \right) \right|}{x} \right)^{\frac{1}{n-1}}.$$

Then,

$$f'(x) = 1 - \frac{\left| \det \left(D_\alpha(G) - \frac{2\alpha W(G)}{n} \right) \right|^{\frac{1}{n-1}}}{x^{\frac{n}{n-1}}} \quad \text{and} \quad f''(x) = \frac{n \left| \det \left(D_\alpha(G) - \frac{2\alpha W(G)}{n} \right) \right|^{\frac{1}{n-1}}}{(n-1)x^{\frac{2n-1}{n-1}}}.$$

In order to calculate the extreme point, we require $f'(x) = 0$. This implies

$$x = \left| \det \left(D_\alpha(G) - \frac{2\alpha W(G)}{n} \right) \right|^{\frac{1}{n}}.$$

At this point,

$$f''(x) = \frac{n}{n-1} \left| \det \left(D_\alpha(G) - \frac{2\alpha W(G)}{n} \right) \right|^{\frac{-1}{n}} \geq 0 \quad \text{for all } n > 1.$$

Therefore, the function $f(x)$ reaches a minimum at $x = \left| \det \left(D_\alpha(G) - \frac{2\alpha W(G)}{n} \right) \right|^{\frac{1}{n}}$, and the minimum value is

$$f \left(\left| \det \left(D_\alpha(G) - \frac{2\alpha W(G)}{n} \right) \right|^{\frac{1}{n}} \right) = n \left| \det \left(D_\alpha(G) - \frac{2\alpha W(G)}{n} \right) \right|^{\frac{1}{n}}.$$

However,

$$\frac{\left| \partial_1 - \frac{2\alpha W(G)}{n} \right| + \dots + \left| \partial_n - \frac{2\alpha W(G)}{n} \right|}{n} \geq \left(\left| \partial_1 - \frac{2\alpha W(G)}{n} \right| \dots \left| \partial_n - \frac{2\alpha W(G)}{n} \right| \right)^{\frac{1}{n}}.$$

Suppose that β is the integer such that $\partial_\beta \geq \frac{2\alpha W(G)}{n}$ and $\partial_{\beta+1} \leq \frac{2\alpha W(G)}{n}$. By Lemma 5, we have

$$\begin{aligned} \frac{\left| \partial_1 - \frac{2\alpha W(G)}{n} \right| + \dots + \left| \partial_n - \frac{2\alpha W(G)}{n} \right|}{n} &\leq \max_{1 \leq i \leq n} \left\{ \frac{\left| \partial_i - \frac{2\alpha W(G)}{n} \right|}{1} \right\} \\ &= \max \left\{ \max_{1 \leq i \leq \beta} \left\{ \partial_i - \frac{2\alpha W(G)}{n} \right\}, \max_{\beta+1 \leq i \leq n} \left\{ \frac{2\alpha W(G)}{n} - \partial_i \right\} \right\} \\ &= \max \left\{ \partial_1 - \frac{2\alpha W(G)}{n}, \frac{2\alpha W(G)}{n} - \partial_n \right\}. \end{aligned}$$

Then, for $\rho_n \geq (2\alpha - 1)\frac{2W(G)}{n}$, and $\alpha \neq 1$, we have

$$\partial_1 - \frac{2\alpha W(G)}{n} \geq \max \left\{ \partial_1 - \frac{2\alpha W(G)}{n}, \frac{2\alpha W(G)}{n} - \partial_n \right\},$$

which implies that

$$\left| \det \left(D_\alpha(G) - \frac{2\alpha W(G)}{n} \right) \right|^{\frac{1}{n}} \leq \max \left\{ \partial_1 - \frac{2\alpha W(G)}{n}, \frac{2\alpha W(G)}{n} - \partial_n \right\}.$$

Therefore, the function $f(x)$ is increasing in the interval

$$\left| \det \left(D_\alpha(G) - \frac{2\alpha W(G)}{n} \right) \right|^{\frac{1}{n}} < \max \left\{ \partial_1 - \frac{2\alpha W(G)}{n}, \frac{2\alpha W(G)}{n} - \partial_n \right\} \leq x,$$

and then

$$f(x) \geq f \left(\max \left\{ \partial_1 - \frac{2\alpha W(G)}{n}, \frac{2\alpha W(G)}{n} - \partial_n \right\} \right).$$

Hence,

$$E^{D_\alpha}(G) \geq \varphi + (n-1) \left(\frac{\left| \det \left(D_\alpha(G) - \frac{2\alpha W(G)}{n} \right) \right|^{\frac{1}{n-1}}}{\varphi} \right),$$

where $\varphi = \max \left\{ \partial_1 - \frac{2\alpha W(G)}{n}, \frac{2\alpha W(G)}{n} - \partial_n \right\}$. The first half of the proof is complete.

Now, suppose equality holds in (8). In this situation,

$$\partial_1 = \max \left\{ \partial_1 - \frac{2\alpha W(G)}{n}, \frac{2\alpha W(G)}{n} - \partial_n \right\} + \frac{2\alpha W(G)}{n}.$$

From equality in (9), we get

$$\sqrt{\left| \partial_2 - \frac{2\alpha W(G)}{n} \right|} = \sqrt{\left| \partial_3 - \frac{2\alpha W(G)}{n} \right|} = \dots = \sqrt{\left| \partial_n - \frac{2\alpha W(G)}{n} \right|},$$

and hence

$$\left(\sum_{i=2}^n \left| \partial_i - \frac{2\alpha W(G)}{n} \right| \right)^2 = (n-1) \left(P - \left(\partial_1 - \frac{2\alpha W(G)}{n} \right)^2 \right),$$

where

$$P = 2(1-\alpha)^2 \sum_{1 \leq i < j \leq n} (d_{ij})^2 + \alpha^2 \sum_{i=1}^n Tr_i^2 - \frac{4\alpha^2 W^2(G)}{n}.$$

Therefore,

$$\left| \partial_i - \frac{2\alpha W(G)}{n} \right| = \sqrt{\frac{P - \left(\partial_1 - \frac{2\alpha W(G)}{n} \right)^2}{n-1}}, \quad i = 2, \dots, n.$$

Hence, $\left| \partial_i - \frac{2\alpha W(G)}{n} \right|$ can have at most two distinct values and we arrive at the following:

- (i) G has only one D_α -eigenvalue. Then, $G \cong K_1$.

- (ii) G has precisely a pair of different D_α -eigenvalues. Thanks to Lemma 6, $G \cong K_n$. Note that $\text{spec}(D_\alpha(K_n)) = \{n-1, \alpha n - 1^{[n-1]}\}$. Hence, if $G \cong K_n$, then

$$\max \left\{ \partial_1 - \frac{2\alpha W(G)}{n}, \frac{2\alpha W(G)}{n} - \partial_n \right\} = (1-\alpha)(n-1), \quad \left| \det \left(D_\alpha(G) - \frac{2\alpha W(G)}{n} \right) \right| = (1-\alpha)^2(n-1)^2,$$

and hence $E^{D_\alpha}(G) = 2(1-\alpha)(n-1)$.

- (iii) G possesses precisely three different D_α -eigenvalues. Therefore,

$$\partial_1 = \max \left\{ \partial_1 - \frac{2\alpha W(G)}{n}, \frac{2\alpha W(G)}{n} - \partial_n \right\} + \frac{2\alpha W(G)}{n}$$

and

$$\left| \partial_i - \frac{2\alpha W(G)}{n} \right| = \sqrt{\frac{P - \left(\max \left\{ \partial_1 - \frac{2\alpha W(G)}{n}, \frac{2\alpha W(G)}{n} - \partial_n \right\} \right)^2}{n-1}}, \quad i = 2, \dots, n.$$

Then, we get that G is a graph with exactly three distinct D_α -eigenvalues, and the result follows. \square

Some well-known special graphs include Hamming graph $H(n, d)$, the complete split graph $CS_{t, n-t}$ and the lexicographic product graph $G[H]$. For $H(n, d)$, its vertex set is represented by X^n with d elements in X . If precisely one coordinate of two vertices are different, then they are adjacent. In particular, $H(n, 2)$ becomes the cube Q_n . The graph $CS_{t, n-t}$ is composed of a clique over t vertices and an independent set of $n-t$ vertices. The vertices in cliques are required to be neighbors of each vertex in the independent set. $G[H]$ has the vertex set $V(G) \times V(H)$ and two vertices are adjacent whenever their first coordinates are adjacent in G or they have the same first coordinate, but their second coordinates are adjacent in H .

Remark 2. Note that there are some graphs that have exactly three or four distinct generalized distance eigenvalues. For example, the star graph, the cycle C_4 , the cycle C_5 , and square of the hypercube of dimension n , Q_n^2 have exactly three distinct generalized distance eigenvalues. In addition, the complete bipartite graph $K_{a,b}$, where $a, b \geq 3$, $a+b=n$, the complete split graph $CS_{t, n-t}$, the complement of an edge $K_n - e$ and the closed fence $C_4[K_2]$ have four different generalized distance eigenvalues.

Although we have given in Remark 2 some special classes of graphs with exactly three and exactly four distinct generalized distance eigenvalues, we were unable to giving a complete characterization of such graphs. It will be an interesting problem to characterize all the connected graphs having precisely three or four distinct generalized distance eigenvalues. Therefore, we leave the following problems:

Problem 1. Characterize all the connected graphs having precisely three different generalized distance eigenvalues.

Problem 2. Characterize all the connected graphs having precisely four different generalized distance eigenvalues.

3. Upper Bounds for $E^{D_\alpha}(G)$

In this section, we obtain some sharp upper bounds for the generalized distance energy $E^{D_\alpha}(G)$ of a connected graph G by using diameter d , minimum degree δ , Wiener's index $W(G)$, as well as transmission degrees. The extremal graphs are characterized accordingly. As an application of our results, we will be able to improve some recently given upper bounds for distance energy and distance signless Laplacian energy of a graph G in [25].

Remark 3. Following [25], we have

$$2 \sum_{1 \leq i < j \leq n} (d_{ij})^2 < \frac{(\sum_{i=1}^n Tr_i)^2}{n}.$$

Also, since

$$\left(\sum_{i=1}^n T_i\right)^2 \leq n \sum_{i=1}^n T_i^2 \text{ and } \left(\sum_{i=1}^n Tr_i\right)^2 \leq n \sum_{i=1}^n Tr_i^2,$$

then we get

$$\begin{aligned} & \sqrt{\frac{2(1-\alpha)^2 \sum_{1 \leq i < j \leq n} (d_{ij})^2 + \alpha^2 \sum_{i=1}^n Tr_i^2 - \frac{4\alpha^2 W^2(G)}{n}}{n}} \\ & < \sqrt{\frac{\frac{(1-\alpha)^2 (\sum_{i=1}^n Tr_i)^2}{n} + \alpha^2 \sum_{i=1}^n Tr_i^2 - \frac{\alpha^2 (\sum_{i=1}^n Tr_i)^2}{n}}{n}} \\ & = \sqrt{\frac{(1-2\alpha) \frac{(\sum_{i=1}^n Tr_i)^2}{n} + \alpha^2 \sum_{i=1}^n Tr_i^2}{n}}. \end{aligned}$$

Hence, if $0 \leq \alpha \leq \frac{1}{2}$, then

$$\begin{aligned} \sqrt{\frac{(1-2\alpha) \frac{(\sum_{i=1}^n Tr_i)^2}{n} + \alpha^2 \sum_{i=1}^n Tr_i^2}{n}} & \leq \sqrt{\frac{(1-2\alpha) \sum_{i=1}^n Tr_i^2 + \alpha^2 \sum_{i=1}^n Tr_i^2}{n}} \\ & = (1-\alpha) \sqrt{\frac{\sum_{i=1}^n Tr_i^2}{n}}. \end{aligned}$$

Theorem 5. Let G be a connected graph of order n . If $0 \leq \alpha \leq \frac{1}{2}$, then

$$E^{D_\alpha}(G) \leq (1-\alpha) \sqrt{\frac{\sum_{i=1}^n Tr_i^2}{n}} + \sqrt{(n-1) \left(P - (1-\alpha)^2 \frac{\sum_{i=1}^n Tr_i^2}{n} \right)}, \quad (10)$$

where $P = 2(1-\alpha)^2 \sum_{1 \leq i < j \leq n} (d_{ij})^2 + \alpha^2 \sum_{i=1}^n Tr_i^2 - \frac{4\alpha^2 W^2(G)}{n}$. Equality holds if and only if either G is a complete graph or G is a graph with exactly three distinct D_α -eigenvalues.

Proof. Applying the Cauchy–Schwarz inequality, we have

$$\left(\sum_{i=2}^n \left| \partial_i - \frac{2\alpha W(G)}{n} \right| \right)^2 \leq (n-1) \left(\sum_{i=2}^n \left(\partial_i - \frac{2\alpha W(G)}{n} \right)^2 \right). \quad (11)$$

Hence,

$$\left(E^{D_\alpha}(G) - \left| \partial_1 - \frac{2\alpha W(G)}{n} \right| \right)^2 \leq (n-1) \left(P - \left(\partial_1 - \frac{2\alpha W(G)}{n} \right)^2 \right).$$

Thus,

$$E^{D_\alpha}(G) \leq \partial_1 - \frac{2\alpha W(G)}{n} + \sqrt{(n-1) \left(P - \left(\partial_1 - \frac{2\alpha W(G)}{n} \right)^2 \right)}.$$

We construct a function

$$f(x) = x + \sqrt{(n-1)(P-x^2)}.$$

It follows from straightforward calculations that the function $f(x)$ monotonically decreases for $x \geq \sqrt{\frac{P}{n}}$. Now, by Lemma 2, Remark 3, and inequality

$$\frac{2W(G)}{n} = \sqrt{\frac{(\sum_{i=1}^n Tr_i)^2}{n^2}} \leq \sqrt{\frac{\sum_{i=1}^n Tr_i^2}{n}},$$

we have

$$\partial_1 \geq \sqrt{\frac{\sum_{i=1}^n Tr_i^2}{n}} \geq (1-\alpha) \sqrt{\frac{\sum_{i=1}^n Tr_i^2}{n}} + \frac{2\alpha W(G)}{n} \geq \sqrt{\frac{P}{n}} + \frac{2\alpha W(G)}{n},$$

and hence

$$x \geq (1-\alpha) \sqrt{\frac{\sum_{i=1}^n Tr_i^2}{n}} \geq \sqrt{\frac{P}{n}}.$$

The first half of the proof is complete.

If the equality holds in (10), we see that

$$\partial_1 = (1-\alpha) \sqrt{\frac{\sum_{i=1}^n Tr_i^2}{n}} + \frac{2\alpha W(G)}{n}.$$

From equality in (11), we get

$$\left| \partial_2 - \frac{2\alpha W(G)}{n} \right| = \left| \partial_3 - \frac{2\alpha W(G)}{n} \right| = \dots = \left| \partial_n - \frac{2\alpha W(G)}{n} \right|,$$

then we have

$$\left| \partial_i - \frac{2\alpha W(G)}{n} \right| = \sqrt{\frac{P - \left(\partial_1 - \frac{2\alpha W(G)}{n} \right)^2}{n-1}}, \quad i = 2, \dots, n.$$

Hence, $\left| \partial_i - \frac{2\alpha W(G)}{n} \right|$ can have no more than a pair of different values and we arrive at the following:

- (i) G has only one D_α -eigenvalue. Then, $G \cong K_1$.
- (ii) G has precisely a pair of different D_α -eigenvalues. Thanks to Lemma 6, $G \cong K_n$.
- (iii) G has precisely three different D_α -eigenvalues. We have

$$\partial_1 = (1-\alpha) \sqrt{\frac{\sum_{i=1}^n Tr_i^2}{n}} + \frac{2\alpha W(G)}{n}, \quad \left| \partial_i - \frac{2\alpha W(G)}{n} \right| = \sqrt{\frac{P - \frac{(1-\alpha)^2 \sum_{i=1}^n Tr_i^2}{n}}{n-1}}, \quad i = 2, \dots, n.$$

Then, we obtain that G is a graph with three distinct D_α -eigenvalues. \square

The following result gives an upper bound for the generalized distance energy $E^{D_\alpha}(G)$ using Wiener's index $W(G)$, diameter d as well as minimum degree δ .

Corollary 1. Let G be connected having n vertices. If $0 \leq \alpha \leq \frac{1}{2}$, then

$$E^{D_\alpha}(G) \leq (1 - \alpha)\sigma + \sqrt{(n - 1)(P - (1 - \alpha)^2\sigma^2)},$$

where $\sigma = dn - \frac{d(d-1)}{2} - 1 - \delta(d-1)$, where the equality holds if and only if either G is a complete graph or G is a graph with precisely three different D_α -eigenvalues.

Proof. A line of calculation shows

$$\begin{aligned} \text{Tr}_p = \sum_{j=1}^n d_{jp} &\leq d_p + 2 + 3 + \cdots + (d-1) + d(n-1-d_p-(d-2)) \\ &= dn - \frac{d(d-1)}{2} - 1 - d_p(d-1), \quad \text{for all } p = 1, 2, \dots, n. \end{aligned} \quad (12)$$

Hence, if $0 \leq \alpha \leq \frac{1}{2}$, then, by Theorem 5, we get

$$\begin{aligned} (1 - \alpha) \sqrt{\frac{\sum_{i=1}^n \text{Tr}_i^2}{n}} &\leq (1 - \alpha) \sqrt{\frac{n \left(dn - \frac{d(d-1)}{2} - 1 - \delta(d-1) \right)^2}{n}} \\ &= (1 - \alpha) \left(dn - \frac{d(d-1)}{2} - 1 - \delta(d-1) \right). \end{aligned}$$

Hence, from the upper bound of Theorem 5, the first part of the proof is done. The rest of the proof follows Theorem 5. \square

Since for any i , we have $n - 1 \leq \text{Tr}_i \leq \frac{n(n-1)}{2}$, hence one can analogously show the following theorem.

Corollary 2. Let G be connected possessing n vertices. If $0 \leq \alpha \leq \frac{1}{2}$, then

$$E^{D_\alpha}(G) \leq S + \sqrt{(n - 1)(P - S^2)},$$

where $S = \frac{n(1-\alpha)(n-1)}{2}$. The equality holds if and only if either G is a complete graph or G is a graph with exactly three distinct D_α -eigenvalues.

Remark 4. If G is connected possessing positive generalized distance eigenvalues, then for $0 \leq \alpha \leq \frac{1}{2}$, we have

$$\frac{2(1 - \alpha)^2 \sum_{1 \leq i < j \leq n} (d_{ij})^2 + \alpha^2 \sum_{i=1}^n \text{Tr}_i^2 - \frac{4\alpha^2 W^2(G)}{n}}{n} \leq \frac{4(1 - \alpha)^2 W^2(G)}{n^2}, \quad (13)$$

since $\sum_{i=1}^n a_i^2 < \frac{2}{n} (\sum_{i=1}^n a_i)^2$, where a_1, \dots, a_n are positive real numbers (see [25]); hence, we get

$$\begin{aligned} 2(1 - \alpha)^2 \sum_{1 \leq i < j \leq n} (d_{ij})^2 + \alpha^2 \sum_{i=1}^n \text{Tr}_i^2 &= \sum_{i=1}^n d_i^2 < \frac{2}{n} \left(\sum_{i=1}^n d_i \right)^2 = \\ \frac{8\alpha^2 W^2(G)}{n} &\leq \frac{4(2\alpha^2 - 2\alpha + 1) W^2(G)}{n} = \frac{4(1 - \alpha)^2 W^2(G)}{n} + \frac{4\alpha^2 W^2(G)}{n}. \end{aligned}$$

Hence, it can be easily seen that the inequality occurs in (13). On the other hand, since $(\sum_{i=1}^n \text{Tr}_i)^2 \leq n \sum_{i=1}^n \text{Tr}_i^2$, we obtain

$$\begin{aligned}
& \sqrt{\frac{2(1-\alpha)^2 \sum_{1 \leq i < j \leq n} (d_{ij})^2 + \alpha^2 \sum_{i=1}^n Tr_i^2 - \frac{4\alpha^2 W^2(G)}{n}}{n}} \\
& \geq \sqrt{\frac{2(1-\alpha)^2 \sum_{1 \leq i < j \leq n} (d_{ij})^2 + \frac{\alpha^2 (\sum_{i=1}^n Tr_i)^2}{n} - \frac{\alpha^2 (\sum_{i=1}^n Tr_i)^2}{n}}{n}} \\
& = \sqrt{\frac{2(1-\alpha)^2 \sum_{1 \leq i < j \leq n} (d_{ij})^2}{n}} \geq \sqrt{\frac{2(1-\alpha)^2 \sum_{1 \leq i < j \leq n} d_{ij}}{n}} \geq (1-\alpha) \sqrt{\frac{2W(G)}{n}}.
\end{aligned}$$

Theorem 6. Let G be connected having $n \geq 3$ vertices.

(i) If $\alpha = 0$, then

$$E^D(G) \leq \frac{2W(G)}{n} + \sqrt{\frac{2W(G)}{n}} + \sqrt{(n-2) \left(2 \sum_{1 \leq i < j \leq n} (d_{ij})^2 - \frac{2W(G)}{n} - \frac{4W^2(G)}{n^2} \right)}.$$

(ii) If $0 < \alpha \leq \frac{1}{2}$ and $\partial_n \geq (1-\alpha) \left(\frac{2W(G)}{n} - \sqrt{\frac{2W(G)}{n}} \right)$, then

$$\begin{aligned}
E^{D_\alpha}(G) & \leq \frac{2(1-\alpha)W(G)}{n} + (1-\alpha) \sqrt{\frac{2W(G)}{n}} \\
& \quad + \sqrt{(n-2) \left(P - \frac{2(1-\alpha)^2 W(G)}{n} - \frac{4(1-\alpha)^2 W^2(G)}{n^2} \right)},
\end{aligned}$$

where $P = 2(1-\alpha)^2 \sum_{1 \leq i < j \leq n} (d_{ij})^2 + \alpha^2 \sum_{i=1}^n Tr_i^2 - \frac{4\alpha^2 W^2(G)}{n}$. The equality holds if and only if G possesses precisely three or four different D_α -eigenvalues.

Proof. Invoking the Cauchy–Schwarz inequality, we obtain

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

and then

$$\begin{aligned}
E^{D_\alpha}(G) & \leq \left| \partial_1 - \frac{2\alpha W(G)}{n} \right| + \left| \partial_n - \frac{2\alpha W(G)}{n} \right| \\
& \quad + \sqrt{(n-2) \left(P - \left(\partial_1 - \frac{2\alpha W(G)}{n} \right)^2 - \left(\partial_n - \frac{2\alpha W(G)}{n} \right)^2 \right)},
\end{aligned}$$

where $P = 2(1-\alpha)^2 \sum_{1 \leq i < j \leq n} (d_{ij})^2 + \alpha^2 \sum_{i=1}^n Tr_i^2 - \frac{4\alpha^2 W^2(G)}{n}$. Let $x = \left| \partial_1 - \frac{2\alpha W(G)}{n} \right|$ and $y = \left| \partial_n - \frac{2\alpha W(G)}{n} \right|$. We define the function

$$f(x, y) = x + y + \sqrt{(n-2)(P - x^2 - y^2)}.$$

Taking derivatives on $f(x, y)$ with respect to x and y , we have

$$f_x = 1 - \frac{x(n-2)}{\sqrt{(n-2)(P-x^2-y^2)}}, \quad f_y = 1 - \frac{y(n-2)}{\sqrt{(n-2)(P-x^2-y^2)}},$$

$$f_{xx} = -\frac{(P-y^2)\sqrt{n-2}}{\sqrt{(P-x^2-y^2)^3}}, \quad f_{yy} = -\frac{(P-x^2)\sqrt{n-2}}{\sqrt{(P-x^2-y^2)^3}} \text{ and } f_{xy} = -\frac{xy\sqrt{n-2}}{\sqrt{(P-x^2-y^2)^3}}.$$

In order to calculate the extreme values, we set $f_x = 0$ and $f_y = 0$. This yields $x = y = \sqrt{\frac{P}{n}}$. At this point, the values of f_{xx}, f_{yy}, f_{xy} and $\Delta = f_{xx}f_{yy} - f_{xy}^2$ are

$$f_{xx} = -\frac{(n-1)\sqrt{n-2}}{\sqrt{\frac{P(n-2)^3}{n}}} \leq 0, \quad f_{yy} = -\frac{(n-1)\sqrt{n-2}}{\sqrt{\frac{P(n-2)^3}{n}}} \leq 0,$$

$$f_{xy} = -\frac{\sqrt{n-2}}{\sqrt{\frac{P(n-2)^3}{n}}} \leq 0 \text{ and } \Delta = \frac{n(n^2-3n+3)}{P(n-2)^2} \geq 0.$$

Hence, $f(x, y)$ has maximum value at this point, and accordingly $f\left(\sqrt{\frac{P}{n}}, \sqrt{\frac{P}{n}}\right) = \sqrt{nP}$. Nevertheless, $f(x, y)$ decreases in the intervals

$$\sqrt{\frac{P}{n}} \leq x \leq \sqrt{\frac{P}{2}} \text{ and } 0 \leq y \leq \sqrt{\frac{P}{n}} \leq \sqrt{\frac{P}{2}}.$$

We examine the following two situations:

- (i) If $\alpha = 0$, then as $2\sum_{1 \leq i < j \leq n} (d_{ij})^2 < \frac{(\sum_{i=1}^n Tr_i)^2}{n}$ (see [25]), we obtain

$$\sqrt{\frac{P}{n}} = \sqrt{\frac{2\sum_{1 \leq i < j \leq n} (d_{ij})^2}{n}} < \sqrt{\frac{(\sum_{i=1}^n Tr_i)^2}{n^2}} = \frac{2W(G)}{n}.$$

In addition, we obtain

$$\sqrt{\frac{P}{n}} = \sqrt{\frac{2\sum_{1 \leq i < j \leq n} (d_{ij})^2}{n}} \geq \sqrt{\frac{2\sum_{1 \leq i < j \leq n} (d_{ij})}{n}} = \sqrt{\frac{2W(G)}{n}}.$$

Hence,

$$\sqrt{\frac{P}{n}} \leq \frac{2W(G)}{n} \leq x \leq \sqrt{\frac{P}{2}} \text{ and } 0 \leq y \leq \sqrt{\frac{2W(G)}{n}} \leq \sqrt{\frac{P}{n}}.$$

Then,

$$f(x, y) \leq f\left(\frac{2W(G)}{n}, \sqrt{\frac{2W(G)}{n}}\right) \leq f\left(\sqrt{\frac{P}{n}}, \sqrt{\frac{P}{n}}\right).$$

Therefore,

$$E^{D_0}(G) \leq \frac{2W(G)}{n} + \sqrt{\frac{2W(G)}{n}} + \sqrt{(n-2) \left(2 \sum_{1 \leq i < j \leq n} (d_{ij})^2 - \frac{2W(G)}{n} - \frac{4W^2(G)}{n^2} \right)}.$$

(ii) If $0 < \alpha \leq \frac{1}{2}$, then, by Remark 4, as $\partial_1 \geq \partial_2 \geq \dots \geq \partial_n > 0$, we have

$$\sqrt{\frac{P}{n}} \leq \frac{2(1-\alpha)W(G)}{n} \leq x \leq \sqrt{\frac{P}{2}}.$$

Again by Remark 4 and as $\partial_n \geq (1-\alpha) \left(\frac{2W(G)}{n} - \sqrt{\frac{2W(G)}{n}} \right)$, we get

$$0 \leq y \leq (1-\alpha) \sqrt{\frac{2W(G)}{n}} \leq \sqrt{\frac{P}{n}}.$$

Then,

$$f(x, y) \leq f\left(\frac{2(1-\alpha)W(G)}{n}, (1-\alpha) \sqrt{\frac{2W(G)}{n}}\right) \leq f\left(\sqrt{\frac{P}{n}}, \sqrt{\frac{P}{n}}\right).$$

Therefore,

$$\begin{aligned} E^{D_\alpha}(G) &\leq \frac{2(1-\alpha)W(G)}{n} + (1-\alpha) \sqrt{\frac{2W(G)}{n}} \\ &\quad + \sqrt{(n-2) \left(P - \frac{2(1-\alpha)^2 W(G)}{n} - \frac{4(1-\alpha)^2 W^2(G)}{n^2} \right)}. \end{aligned}$$

The rest of the proof follows from Theorem 4. \square

Remark 5. Keeping all of the notations from Theorem 6, and taking

$$h(x, y) = x + y + \sqrt{(n-1)(P - x^2 - y^2)},$$

then it is clear that $f(x, y) \leq h(x, y)$ for all (x, y) in the given region of x and y . For $0 \leq \alpha \leq \frac{1}{2}$, along $x = \frac{2(1-\alpha)W(G)}{n}$,

$$f(x, y) = \frac{2(1-\alpha)W(G)}{n} + y + \sqrt{(n-2) \left(P - \frac{4(1-\alpha)^2 W^2(G)}{n^2} - y^2 \right)},$$

where $P = 2(1-\alpha)^2 \sum_{1 \leq i < j \leq n} (d_{ij})^2 + \alpha^2 \sum_{i=1}^n \text{Tr}_i^2 - \frac{4\alpha^2 W^2(G)}{n}$. The function $f\left(\frac{2(1-\alpha)W(G)}{n}, y\right)$ decreases in the interval $0 \leq y \leq \sqrt{P - \frac{4(1-\alpha)^2 W^2(G)}{n^2}}$. By Remark 4, we have

$$2(1-\alpha)^2 W(G) \leq P \leq \frac{4(1-\alpha)^2 W^2(G)}{n},$$

hence as $P \geq \frac{8(1-\alpha)^2 W^2(G)}{n^2} \geq 2(1-\alpha)^2 W(G)$, we have

$$0 \leq y \leq (1-\alpha) \sqrt{\frac{2W(G)}{n}} \leq \sqrt{P - \frac{4(1-\alpha)^2 W^2(G)}{n^2}}.$$

Thus,

$$f\left(\frac{2(1-\alpha)W(G)}{n}, (1-\alpha) \sqrt{\frac{2W(G)}{n}}\right) \leq f\left(\frac{2(1-\alpha)W(G)}{n}, 0\right).$$

Since

$$f\left(\frac{2(1-\alpha)W(G)}{n}, 0\right) \leq h\left(\frac{2(1-\alpha)W(G)}{n}, 0\right)$$

and

$$h\left(\frac{2(1-\alpha)W(G)}{n}, 0\right) = \frac{2(1-\alpha)W(G)}{n} + \sqrt{(n-1)\left(P - \frac{4(1-\alpha)^2W^2(G)}{n^2}\right)},$$

then

$$f\left(\frac{2(1-\alpha)W(G)}{n}, (1-\alpha)\sqrt{\frac{2W(G)}{n}}\right) \leq h\left(\frac{2(1-\alpha)W(G)}{n}, 0\right).$$

Hence,

$$\begin{aligned} & \frac{2(1-\alpha)W(G)}{n} + (1-\alpha)\sqrt{\frac{2W(G)}{n}} + \sqrt{(n-2)\left(P - \frac{2(1-\alpha)^2W(G)}{n} - \frac{4(1-\alpha)^2W^2(G)}{n^2}\right)} \\ & \leq \frac{2(1-\alpha)W(G)}{n} + \sqrt{(n-1)\left(P - \frac{4(1-\alpha)^2W^2(G)}{n^2}\right)}. \end{aligned}$$

The following upper bound was proved in in [25]:

$$E^D(G) \leq \frac{2W(G)}{n} + \sqrt{(n-1)\left(2 \sum_{1 \leq i < j \leq n} (d_{ij})^2 - \frac{4W^2(G)}{n^2}\right)}. \quad (14)$$

Remark 6. For $\alpha = 0$, it is easily seen by Remark 5 that the upper bound in Theorem 6 improves that presented in (14).

In addition, the following upper bound for the distance signless Laplacian energy $E^Q(G)$ was obtained in [25]:

$$E^Q(G) \leq \frac{2W(G)}{n} + \sqrt{(n-1)\left(2 \sum_{1 \leq i < j \leq n} (d_{ij})^2 + \sum_{i=1}^n \text{Tr}_i^2 - \frac{4W^2(G)}{n} - \frac{4W^2(G)}{n^2}\right)}. \quad (15)$$

Remark 7. For $\alpha = \frac{1}{2}$, it is not difficult to see by Remark 5 that the upper bound shown in Theorem 6 improves that presented in (15).

We recall the following lemma.

Lemma 7 (Theorem 2.11 [8]). Let G have $n > 1$ vertices. For the largest and second largest generalized distance eigenvalues ∂_1 and ∂_2 of G , we have

$$\partial_1 + \partial_2 \leq \frac{4\alpha W(G) + \sqrt{2(8\alpha^2 W^2(G) - n(4\alpha^2 W^2(G) - K(n-2)))}}{n},$$

where $K = 2(1-\alpha)^2 \sum_{1 \leq i < j \leq n} (d_{ij})^2 + \alpha^2 \sum_{i=1}^n \text{Tr}_i^2$. Equality holds if and only if G is a graph with exactly three or exactly four distinct D_α -eigenvalues.

We conclude with the following upper bound by using only the Wiener index $W(G)$.

Theorem 7. Let G be connected having $n > 1$ vertices. If $\partial_2 \geq \frac{2\alpha W(G)}{n}$, then

$$E^{D_\alpha}(G) \leq \frac{\sqrt{2(8\alpha^2 W^2(G) - n(4\alpha^2 W^2(G) - K(n-2)))}}{n} + \sqrt{P(n-2)}, \quad (16)$$

where $K = 2(1 - \alpha)^2 \sum_{1 \leq i < j \leq n} (d_{ij})^2 + \alpha^2 \sum_{i=1}^n \text{Tr}_i^2$ and $P = K - \frac{4\alpha^2 W^2(G)}{n}$. The equality holds if and only if G is a graph with precisely three or four different D_α -eigenvalues.

Proof. Thanks to the Cauchy–Schwarz inequality, we obtain

$$\left(\sum_{i=3}^n \left| \partial_i - \frac{2\alpha W(G)}{n} \right| \right)^2 \leq \left(\sum_{i=3}^n 1 \right) \left(\sum_{i=3}^n \left| \partial_i - \frac{2\alpha W(G)}{n} \right|^2 \right).$$

Then,

$$\begin{aligned} E^{D_\alpha}(G) &\leq \left| \partial_1 - \frac{2\alpha W(G)}{n} \right| + \left| \partial_2 - \frac{2\alpha W(G)}{n} \right| \\ &\quad + \sqrt{(n-2) \left(P - \left(\left(\partial_1 - \frac{2\alpha W(G)}{n} \right)^2 + \left(\partial_2 - \frac{2\alpha W(G)}{n} \right)^2 \right) \right)}, \end{aligned}$$

where $P = 2(1 - \alpha)^2 \sum_{1 \leq i < j \leq n} (d_{ij})^2 + \alpha^2 \sum_{i=1}^n \text{Tr}_i^2 - \frac{4\alpha^2 W^2(G)}{n}$. Hence, by Lemma 7, we get

$$\begin{aligned} E^{D_\alpha}(G) &\leq \frac{\sqrt{2(8\alpha^2 W^2(G) - n(4\alpha^2 W^2(G) - K(n-2)))}}{n} \\ &\quad + \sqrt{(n-2) \left(P - \left(\left(\partial_1 - \frac{2\alpha W(G)}{n} \right)^2 + \left(\partial_2 - \frac{2\alpha W(G)}{n} \right)^2 \right) \right)}, \end{aligned}$$

where $K = 2(1 - \alpha)^2 \sum_{1 \leq i < j \leq n} (d_{ij})^2 + \alpha^2 \sum_{i=1}^n \text{Tr}_i^2$. Construct a function

$$f(x, y) = \frac{\sqrt{2(8\alpha^2 W^2(G) - n(4\alpha^2 W^2(G) - K(n-2)))}}{n} + \sqrt{(n-2)(P - (x^2 + y^2))}.$$

Taking derivatives on $f(x, y)$ regarding x and y , we have

$$\begin{aligned} f_x &= -\frac{x\sqrt{n-2}}{\sqrt{P - (x^2 + y^2)}}, \quad f_y = -\frac{y\sqrt{n-2}}{\sqrt{P - (x^2 + y^2)}}, \\ f_{xx} &= -\frac{(P - y^2)\sqrt{n-2}}{\sqrt{(P - (x^2 + y^2))^3}}, \quad f_{yy} = -\frac{(P - x^2)\sqrt{n-2}}{\sqrt{(P - (x^2 + y^2))^3}}, \quad f_{xy} = -\frac{xy\sqrt{n-2}}{\sqrt{(P - (x^2 + y^2))^3}}. \end{aligned}$$

In order to calculate the extreme points, we set $f_x = 0$ and $f_y = 0$. This yields $x = y = 0$. At this point, the values of f_{xx}, f_{yy}, f_{xy} and $\Delta = f_{xx}f_{yy} - f_{xy}^2$ are $f_{xx} = -\sqrt{\frac{n-2}{P}}, f_{yy} = -\sqrt{\frac{n-2}{P}}, f_{xy} = 0$ and $\Delta = f_{xx}f_{yy} - (f_{xy})^2 = \frac{n-2}{P} \geq 0$. Then, $f(x, y)$ attains maximum value at $x = y = 0$, hence

$$f(0, 0) = \frac{\sqrt{2(8\alpha^2 W^2(G) - n(4\alpha^2 W^2(G) - K(n-2)))}}{n} + \sqrt{P(n-2)}.$$

Thus,

$$E^{D_\alpha}(G) \leq \frac{\sqrt{2(8\alpha^2 W^2(G) - n(4\alpha^2 W^2(G) - K(n-2)))}}{n} + \sqrt{P(n-2)}.$$

The rest of the proof follows similarly as Theorem 4. \square

4. Conclusions

The notion of generalized distance energy of a graph G was first motivated in Alhevaz et al. [17] as the average deviation of generalized distance spectrum:

$$E^{D_\alpha}(G) = \sum_{i=1}^n \left| d_i - \frac{2\alpha W(G)}{n} \right|,$$

where $W(G)$ is Wiener's index. Arguably, the distance and the distance signless Laplacian play a pivotal role in mathematics as they offer more information than the classical binary adjacency matrix. In this work, we along this line further investigate the energy of a generalized distance matrix. It forms a natural extension of the theory of distance energy as well as distance signless Laplacian energy. The spectral properties of these relevant individual combinatorial matrices can be derived as special situations in the framework of a generalized distance matrix. We developed some properties of $E^{D_\alpha}(G)$ by establishing new inequalities including sharp upper and lower bounds linking a range of invariants such as diameter, extreme degree, Wiener's index as well as transmission degrees. Existing bounds in the literature have been improved and extremal graphs have been determined. For future work, it would be desirable to derive some other sharp bounds for the generalized distance energy leveraging a variety of graph invariants.

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