mathematics

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Merging the Spectral Theories of Distance Estrada and Distance Signless Laplacian Estrada Indices of Graphs

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Received: 14 August 2019; Accepted: 16 October 2019; Published: 19 October 2019

Abstract: Suppose that G is a simple undirected connected graph. Denote by $D(G)$ the distance matrix of G and by $Tr(G)$ the diagonal matrix of the vertex transmissions in G, and let $\alpha \in [0,1]$. The generalized distance matrix $D_\alpha(G)$ is defined as $D_\alpha(G) = \alpha Tr(G) + (1-\alpha)D(G)$, where $0 \leq \alpha \leq 1$. If $\partial_1 \geq \partial_2 \geq \ldots \geq \partial_n$ are the eigenvalues of $D_\alpha(G)$; we define the generalized distance Estrada index of the graph G as $D_\alpha E(G) = \sum_{i=1}^{n} e^{\left(\partial_i - \frac{2\alpha W(G)}{n}\right)}$, where $W(G)$ denotes for the Wiener index of G. It is clear from the definition that $D_0E(G) = DEE(G)$ and $2D_{\frac{1}{2}}E(G) = D^QEE(G)$, where $DEE(G)$ denotes the distance Estrada index of G and $D^QEE(G)$ denotes the distance signless Laplacian Estrada index of G. This shows that the concept of generalized distance Estrada index of a graph G merges the theories of distance Estrada index and the distance signless Laplacian Estrada index. In this paper, we obtain some lower and upper bounds for the generalized distance Estrada index, in terms of various graph parameters associated with the structure of the graph G, and characterize the extremal graphs attaining these bounds. We also highlight relationship between the generalized distance Estrada index and the other graph-spectrum-based invariants, including generalized distance energy. Moreover, we have worked out some expressions for $D_\alpha E(G)$ of some special classes of graphs.

Keywords: generalized distance matrix (spectrum); distance (signless Laplacian) Estrada index; distance (signless Laplacian) matrix; generalized distance Estrada index; generalized distance energy

MSC: 05C50, 05C12, 15A18

1. Introduction

In this paper, we are concerned only with simple, finite, connected and undirected graphs with vertex set $V(G) = \{v_1, v_2, \ldots, v_n\}$ and edge set $E(G)$. The *order* and the *size* of G is, respectively, the number of vertices and the number of edges of G. The *degree* of a vertex v, denoted by $d_G(v)$ (or simply d_v) is the cardinality of the set of vertices adjacent to v in a graph G. The *distance* between two vertices $u, v \in V(G)$, denoted by d_{uv}, represents the number of edges in a shortest path between these two end nodes in G. The *diameter* of G is the maximum distance between any pair of vertices of G. The *distance matrix* $D(G)$ of a graph G is a square symmetric matrix defined as $D(G) = (d_{uv})_{u,v \in V(G)}$. The *transmission* of a vertex v, denoted by $Tr_G(v)$, is defined as the sum of the distances from v to all other vertices in G, in other words, $Tr_G(v) = \sum\limits_{u \in V(G)} d_{uv}$. A graph G is referred to as *k-transmission regular* when the matrix $D(G)$ has the constant row sum equal to k. The *Wiener index* (also called the *transmission*) of a graph G, denoted by $W(G)$, is the sum of distances between all unordered pairs of vertices in G. Apparently, $W(G) = \frac{1}{2} \sum_{v \in V(G)} Tr_G(v)$. For any vertex $v_i \in V(G)$, the transmission $Tr_G(v_i)$ is also called the *transmission degree*, shortly denoted by Tr_i, and the sequence $\{Tr_1, Tr_2, \ldots, Tr_n\}$ is called the *transmission degree sequence* of the graph G.

Let $Tr(G) = diag(Tr_1, Tr_2, \ldots, Tr_n)$ be the diagonal matrix of vertex transmissions of G. Following Aouchiche and Hansen [1,2], the *distance Laplacian matrix* and the *distance signless Laplacian matrix* of a graph G are defined, respectively, as $D^L(G) = Tr(G) - D(G)$ and $D^Q(G) = Tr(G) + D(G)$. Recently, the spectral properties of the distance Laplacian matrix, distance matrix, as well as distance signless Laplacian matrix have attracted attention of the many researchers and a large number of papers have been published regarding their spectral properties, like spectral radius, energy, Estrada index, second largest eigenvalue, smallest eigenvalue, etc. For some recent works, we refer to [3–5] and the references cited therein.

Motivated by [6], Cui et al. [7] introduced the *generalized distance matrix* $D_\alpha(G)$ as a convex combinations of $Tr(G)$ and $D(G)$, defined as $D_\alpha(G) = \alpha Tr(G) + (1-\alpha)D(G)$, for $0 \leq \alpha \leq 1$. Noting that $D_0(G) = D(G), 2D_{\frac{1}{2}}(G) = D^Q(G), D_1(G) = Tr(G)$, and $D_\alpha(G) - D_\beta(G) = (\alpha - \beta)D^L(G)$, any result regarding the spectral properties of generalized distance matrix has its counterpart for each of these particular graph matrices, and these counterparts following immediately from a single proof. In fact, this matrix reduces to merging the distance Laplacian spectral, distance spectral, as well as distance signless Laplacian spectral theories. As the matrix $D_\alpha(G)$ is real symmetric, all its eigenvalues are real. Therefore, we can arrange them as $\partial_1 \geq \partial_2 \geq \cdots \geq \partial_n$. The largest eigenvalue ∂_1 of the matrix $D_\alpha(G)$ is called the *generalized distance spectral radius* of G (We will denote $\partial_1(G)$ by $\partial(G)$).

Based upon some geometric characteristics of biomolecules, Ernesto Estrada [8,9] investigated an expression taking the form

$$EE(G) = \sum_{i=1}^{n} e^{\lambda_i},$$

where $\lambda_1, \lambda_2, \ldots, \lambda_n$ represent all eigenvalues of the adjacency matrix of a molecular graph G. Analytical studies on this quantity was performed later in [10] and the name "Estrada index" was proposed in [11]. The properties of the Estrada index have been intensively explored, see, for example [11–14]. There exists a vast literature related to Estrada index and its bounds and we refer the reader to the nice surveys [15,16].

This graph-spectrum-based invariant has also an important role in chemistry, biology, as well as network science. It has been applied for instance to gauge the extent of folding of long chain polymeric molecules, encompassing some proteins [8,17,18]. It has found a number of applications in complex networks and characterizes the centrality [9]. EE offers a unique metric to characterize the robustness of complex networks [19]; namely, it is a monotonic measure with respect to the edge deletion and addition. For more applications of the Estrada index in network science, see the monograph in [20] and papers [19,21].

The pioneering papers [8,9] further investigate varied versions of Estrada index with respect to other graph associated matrices. Because of the evident success of the graph Estrada index, this proposal has been put into effect, and Estrada index-based on the eigenvalues of more graph matrices have been introduced subsequently: Estrada index-based invariant with respect to distance matrix [22], Estrada index-based invariant with respect to Laplacian matrix [23,24], Estrada index-based invariant with respect to signless Laplacian matrix [25,26], and Estrada index-based invariant with respect to distance signless Laplacian matrix [27] have been introduced and studied. For some other interesting papers, we direct the reader to works [28–31].

The distance matrix graph has shown its importance in a wide range of areas across science and engineering. The distance matrix contains information on the number of walks and self-avoiding walks of chemical graphs, which adjacency matrix fails to show. Distance matrix has been used to calculate many topological indices, including the Wiener index, and thermodynamic properties involving temperature and pressure coefficients. In the design of communication infrastructure network, molecular stability, and graph embedding theory, distance matrix has played an important role. Distance eigenvalues of graphs have attracted huge attention for mathematicians for decades. For more information regarding distance spectrum, we refer to the survey [1] and the references therein.

We observe that the distance matrix and its eigenvalues are of importance not only from a chemistry point of view, but also because they are very useful in other branches of science and social science. Clearly, the information one gets regarding the graph from the distance matrix is also visible from the distance Laplacian and the distance signless Laplacian matrices of a graph. As these matrices use more structural properties of a graph than the distance matrix, these matrices may contain a wealth of information about the graph. In addition to its formal analogy to the Estrada index, the distance and the distance signless Laplacian Estrada indices are arguably of prominent significance in physical chemistry. Distance turns out to be rooted deeply in the molecular graphs.

Therefore, here we define the *generalized distance Estrada index* $D_\alpha E(G)$, based on the generalized distance matrix of the graph G, as

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

where $\partial_1 \geq \partial_2 \geq \cdots \geq \partial_n$ are the eigenvalues of $D_\alpha(G)$ (the generalized distance eigenvalues of a graph G).

It follows from the definition that $D_0 E(G) = DEE(G)$ and $2D_{1/2}E(G) = D^Q EE(G)$, where $DEE(G)$ denotes the distance Estrada index of a graph G and $D^Q EE(G)$ denotes the distance signless Laplacian Estrada index of a graph G. This shows that the concept of generalized distance Estrada index of a graph G merges the theories of distance Estrada index and the distance signless Laplacian Estrada index of a graph G. Let

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

Then, $U_0 = n, U_1 = 0$ and $U_2 = 2(1-\alpha)^2 \sum_{1\leq i<j\leq n} (d_{ij})^2 + \alpha^2 \sum_{i=1}^{n} Tr_i^2 - \frac{4\alpha^2 W^2(G)}{n}$. Recalling the power series expansion of e^x, we can write the generalized distance Estrada index as

$$D_\alpha E(G) = \sum_{k\geq 0} \frac{U_k}{k!}. \tag{2}$$

The rest of the paper is structured as follows. In Section 2, we mention some preliminary results which will be helpful throughout the paper. In Section 3, we obtain some lower bounds for the generalized distance Estrada index $D_\alpha E(G)$, in terms of various graph parameters associated with structure of the graph G, and identify the extremal graphs attaining these bounds. In Section 4, we obtain some upper bounds for the generalized distance Estrada index $D_\alpha E(G)$ and delineate the extremal graphs. In Section 5, we derive some relations between the generalized distance Estrada index and the generalized distance energy of G. Finally, in Section 6, we obtain some results about generalized distance Estrada index of some elementary graphs and give an expression for $D_\alpha E(G)$ of a (transmission) regular graph G, in terms of the distance eigenvalues as well as adjacency eigenvalues of G, and describe the generalized distance Estrada index of some graphs obtained by operations.

2. Preliminary Results

In this section, we give some preliminary results which will be utilized in the subsequent sections. The following lemma can be found in [7].

Lemma 1 ([7]). *Suppose that G is a connected graph of order n. We have*

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

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

By a similar way as used in the proof of ([32], Lemma 2), we can prove the following lemma.

Lemma 2. *A connected graph G admits two distinct generalized distance eigenvalues if and only if G is a complete graph.*

The proof of the following lemma is similar to that of ([4], Theorem 2.2) and is omitted here.

Lemma 3. *Let the transmission degree sequence of G be $\{Tr_1, Tr_2, \ldots, Tr_n\}$. Then,*

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

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

Given two nonincreasing real sequences $(x) = (x_1, x_2, \ldots, x_n)$ and $(y) = (y_1, y_2, \ldots, y_n)$ of length n, (x) is said to be majorized by (y) or (y) majorizes (x), denoted by $(x) \preceq (y)$ if

$$\sum_{i=1}^{n} x_i = \sum_{i=1}^{n} y_i \quad \text{and} \quad \sum_{i=1}^{k} x_i \leq \sum_{i=1}^{k} y_i, \quad \text{for all } \; k = 1, 2, \ldots, n-1.$$

The relation $(x) \prec (y)$ means that $(x) \preceq (y)$ and (x) is not the rearrangement of (y).

The following observation can be found in [23].

Lemma 4 ([23]). *Let $(x) = (x_1, x_2, \ldots, x_n)$ and $(y) = (y_1, y_2, \ldots, y_n)$ be nonincreasing sequences of real numbers of length n. If $(x) \preceq (y)$, then for any convex function ψ, we have $\sum_{i=1}^{n} \psi(x_i) \leq \sum_{i=1}^{n} \psi(y_i)$. Equality holds if and only if $x_i = y_i$ for all $i = 1, 2, \ldots, n$. In addition, when $(x) \prec (y)$ and ψ is strictly convex, $\sum_{i=1}^{n} \psi(x_i) < \sum_{i=1}^{n} \psi(y_i)$ holds.*

The majorization relation between the spectrum and diagonal elements of Hermitian matrices perfectly links the spectrum of a generalized distance matrix $D_\alpha(G)$ with majorization. The relation given below immediately follows.

Lemma 5. *Assume that G is a connected graph of order n admitting generalized distance eigenvalues $\partial_1, \partial_2, \ldots, \partial_n$ and transmission degrees $Tr_1, Tr_2, \ldots, Tr_n$. Then,*

$$(\alpha Tr_1, \alpha Tr_2, \ldots, \alpha Tr_n) \preceq (\partial_1, \partial_2, \ldots, \partial_n).$$

Theorem 1. *Assume that G is any connected graph of order $n \geq 2$ with transmission degree sequence $\{Tr_1, Tr_2, \ldots, Tr_n\}$.*
(i) *If $k < 0$ or $k > 1$, then $U_k \geq \sum_{i=1}^{n} \left(\alpha Tr_i - \frac{2\alpha W(G)}{n}\right)^k$;*
(ii) *If $0 < k < 1$, then $U_k \leq \sum_{i=1}^{n} \left(\alpha Tr_i - \frac{2\alpha W(G)}{n}\right)^k$.*
Equality occurs in both parts, if and only if $\partial_i = \alpha Tr_i$, for $i = 1, 2, \ldots, n$.

Proof. (i) For $x > 0$, it follows that the function $f(x) = x^k$ is a convex function if $k < 0$ or $k > 1$. Let $(X) = \left(\alpha Tr_1 - \frac{2\alpha W(G)}{n}, \alpha Tr_2 - \frac{2\alpha W(G)}{n}, \ldots, \alpha Tr_n - \frac{2\alpha W(G)}{n}\right)$ and $(Y) = \left(\partial_1 - \frac{2\alpha W(G)}{n}, \partial_2 - \frac{2\alpha W(G)}{n}, \ldots, \partial_n - \frac{2\alpha W(G)}{n}\right)$. By Lemma 5, we have $(X) \preceq (Y)$. It then follows by Lemma 4 that

$$U_k = \sum_{i=1}^{n} \left(\partial_i - \frac{2\alpha W(G)}{n}\right)^k \geq \sum_{i=1}^{n} \left(\alpha Tr_i - \frac{2\alpha W(G)}{n}\right)^k. \tag{3}$$

Therefore, by Lemma 4, equality occurs in the inequality (3) if and only if $(X) = (Y)$. That is, if and only if $\partial_i = \alpha Tr_i$, for all $i = 1, 2, \ldots, n$.
(ii) For $x > 0$, it follows that the function $f(x) = -x^k$ is a convex function if $0 < k < 1$. Therefore, proceeding similarly as in part (i), we arrive at part (ii). □

3. Lower Bounds for the Generalized Distance Estrada Index of Graphs

In this section, we obtain some lower bounds for the generalized distance Estrada index $D_\alpha E(G)$ of a connected graph G. These bounds are characterized in terms of the order n, the Wiener index $W(G)$, the transmission degree and the parameter $\alpha \in [0,1]$. We also investigate the extremal graph attaining these bounds.

Our first result gives a lower bound for the generalized distance Estrada index $D_\alpha E(G)$, in terms of the order n, the transmission degrees and the parameter α.

Theorem 2. *Suppose G is a connected graph of order n. Then,*

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

with equality if and only if $G \cong K_1$.

Proof. Starting with Equation (1), we have

$$D_\alpha E^2(G) = \sum_{i=1}^{n} e^{2\left(\partial_i - \frac{2\alpha W(G)}{n}\right)} + 2\sum_{i<j} e^{\left(\partial_i - \frac{2\alpha W(G)}{n}\right)} e^{\left(\partial_j - \frac{2\alpha W(G)}{n}\right)}. \tag{5}$$

Thanks to the arithmetic–geometric mean inequality, we have

$$
\begin{aligned}
2\sum_{i<j} e^{\left(\partial_i-\frac{2\alpha W(G)}{n}\right)} e^{\left(\partial_j-\frac{2\alpha W(G)}{n}\right)} &\geq n(n-1)\left(\prod_{i>j} e^{(\partial_i-\frac{2\alpha W(G)}{n})} e^{(\partial_j-\frac{2\alpha W(G)}{n})}\right)^{\frac{2}{n(n-1)}} \\
&= n(n-1)\left[\left(\prod_{i=1}^{n} e^{(\partial_i-\frac{2\alpha W(G)}{n})}\right)^{n-1}\right]^{\frac{2}{n(n-1)}} \\
&= n(n-1)(e^{U_1})^{\frac{2}{n}} \\
&= n(n-1). \qquad (6)
\end{aligned}
$$

Using a power-series expansion, and as $U_0 = n$, $U_1 = 0$ and $U_2 = 2(1-\alpha)^2\sum_{1\leq i<j\leq n} d_{ij}^2 + \alpha^2\sum_{i=1}^{n} Tr_i^2 - \frac{4\alpha^2 W^2(G)}{n}$, we get

$$
\begin{aligned}
\sum_{i=1}^{n} e^{2(\partial_i-\frac{2\alpha W(G)}{n})} &= \sum_{i=1}^{n}\sum_{k\geq 0}\frac{\left[2\left(\partial_i-\frac{2\alpha W(G)}{n}\right)\right]^k}{k!} = n + 4(1-\alpha)^2\sum_{1\leq i<j\leq n}(d_{ij})^2 + 2\alpha^2\sum_{i=1}^{n} Tr_i^2 \\
&- \frac{8\alpha^2 W^2(G)}{n} + \sum_{i=1}^{n}\sum_{k\geq 3}\frac{\left[2\left(\partial_i-\frac{2\alpha W(G)}{n}\right)\right]^k}{k!}.
\end{aligned}
$$

We apply a multiplier $r \geq 2$ to arrive at

$$
\begin{aligned}
\sum_{i=1}^{n} e^{2(\partial_i-\frac{2\alpha W(G)}{n})} &\geq n + 4(1-\alpha)^2\sum_{1\leq i<j\leq n}(d_{ij})^2 + 2\alpha^2\sum_{i=1}^{n} Tr_i^2 - \frac{8\alpha^2 W^2(G)}{n} \\
&+ r\sum_{i=1}^{n}\sum_{k\geq 3}\frac{\left(\partial_i-\frac{2\alpha W(G)}{n}\right)^k}{k!} = n + 4(1-\alpha)^2\sum_{1\leq i<j\leq n}(d_{ij})^2 + 2\alpha^2\sum_{i=1}^{n} Tr_i^2 \\
&- \frac{8\alpha^2 W^2(G)}{n} - rn - r(1-\alpha)^2\sum_{1\leq i<j\leq n}(d_{ij})^2 - \frac{r\alpha^2}{2}\sum_{i=1}^{n} Tr_i^2 + \frac{2r\alpha^2 W^2(G)}{n} \\
&+ rD_\alpha E(G) = (1-r)n + \frac{2\alpha^2 W^2(G)}{n}(r-4) + (4-r)(1-\alpha)^2\sum_{1\leq i<j\leq n}(d_{ij})^2 \\
&+ \left(2-\frac{r}{2}\right)\alpha^2\sum_{i=1}^{n} Tr_i^2 + rD_\alpha E(G), \qquad (7)
\end{aligned}
$$

where we have used the fact that $g(x) := e^{2x} - 1 - 2x - 2x^2 - r(e^x - 1 - x - \frac{x^2}{2}) \geq 0$ for $r \geq 2$ since $g(0) = 0$, $g'(x) \leq 0$ for $x \leq 0$ and $g'(x) \geq 0$ for $x \geq 0$ when $r \geq 2$.

Let $P = \sum_{i=1}^{n} Tr_i^2 - \frac{4W^2(G)}{n}$. By substituting (6) and (7) in (5), and solving it for $D_\alpha E(G)$, we get

$$
D_\alpha E(G) \geq \frac{1}{2}\left(r + \sqrt{(r-2n)^2 + 4(4-r)(1-\alpha)^2\sum_{1\leq i<j\leq n}(d_{ij})^2 + 2\alpha^2(4-r)P}\right).
$$

The function

$$f(x) = \frac{1}{2}\left(x + \sqrt{(x-2n)^2 + 4(4-x)(1-\alpha)^2 \sum_{1\leq i<j\leq n}(d_{ij})^2 + 2\alpha^2(4-x)P}\right),$$

monotonically decreases for $x \geq 2$. Consequently, the best lower bound for $D_\alpha E(G)$ is attained for $r = 2$. This gives us the first part of the proof.

From the derivation of (4), we observe readily that the equality holds if and only if G has no non-zero D_α-eigenvalues. Recall that G is connected. Therefore, this can only happen when $G \cong K_1$. The proof is then complete. □

The following result is an immediate consequence of Theorem 2.

Corollary 1. *Assume that G is a connected graph of order n. We have*

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

where the equality holds if and only if $G \cong K_1$.

Proof. As $\sum_{1\leq i<j\leq n}(d_{ij})^2 \geq \frac{n(n-1)}{2}$, from the lower bound of Theorem 2, we obtain

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

Thus, the result, □

The next result gives a complementary lower bound for the generalized distance Estrada index $D_\alpha E(G)$. The bound is characterized by the order n of graph, its Wiener index $W(G)$ as well as the parameter α.

Theorem 3. *Suppose that G is a connected graph of order n. Then,*

$$D_\alpha E(G) \geq e^{\frac{2(1-\alpha)W(G)}{n}} + (n-1)e^{\frac{-2(1-\alpha)W(G)}{n(n-1)}}, \tag{8}$$

where the equality holds if and only if $G = K_n$.

Proof. Thanks to Equation (1) and the well-known arithmetic–geometric mean inequality, we have

$$\begin{aligned} D_\alpha E(G) &= e^{\partial_1 - \frac{2\alpha W(G)}{n}} + e^{\partial_2 - \frac{2\alpha W(G)}{n}} + \cdots + e^{\partial_n - \frac{2\alpha W(G)}{n}} \\ &\geq e^{\partial_1 - \frac{2\alpha W(G)}{n}} + (n-1)\left(\prod_{i=2}^{n} e^{\partial_i - \frac{2\alpha W(G)}{n}}\right)^{\frac{1}{n-1}} \qquad (9) \\ &= e^{\partial_1 - \frac{2\alpha W(G)}{n}} + (n-1)\left(e^{\frac{2\alpha W(G)}{n} - \partial_1}\right)^{\frac{1}{n-1}}. \qquad (10) \end{aligned}$$

Consider the following function,

$$f(x) = e^{x} + (n-1)e^{\frac{-x}{n-1}} \tag{11}$$

for $x \geq 0$. We have

$$f'(x) = e^{x} - e^{\frac{-x}{n-1}} \geq 0$$

for $x \geq 0$. It is not difficult to see that $f(x)$ is increasing for $x \geq 0$. Using Equation (10) and Lemma 1, we obtain

$$D_{\alpha}E(G) \geq e^{\frac{2(1-\alpha)W(G)}{n}} + (n-1)e^{\frac{-2(1-\alpha)W(G)}{n(n-1)}}.$$

Moreover, from the derivation of (8), it is clear that equality holds if and only if the equality holds in the inequality (9). Also, equality holds in (9) if and only if $\partial_2 = \partial_3 = \cdots = \partial_n$. Therefore, G has exactly two distinct generalized distance eigenvalues; then, by Lemma 2, we see that G is the complete graph K_n.

Conversely, it is easy to see that the equality holds in (8) for K_n. □

We will make use of the following lemma in our next results.

Lemma 6 ([33]). *Let $a_1, a_2, \ldots, a_n$ be non-negative numbers. Then,*

$$n\left[\frac{1}{n}\sum_{i=1}^{n} a_i - \left(\prod_{i=1}^{n} a_i\right)^{\frac{1}{n}}\right] \leq n\sum_{i=1}^{n} a_i - \left(\sum_{i=1}^{n} a_i^{\frac{1}{2}}\right)^{2}.$$

Let $M(G) = \left(\prod_{i=1}^{n} Tr_i\right)^{\frac{1}{n}}$ be the geometric mean of the transmission degrees sequence. Clearly, $M(G) \leq \frac{2W(G)}{n}$, and equality is attained if and only if $Tr_1 = Tr_2 = \cdots = Tr_n$ (i.e., G is a transmission regular graph).

Our next result gives a lower bound for $D_{\alpha}E(G)$ in terms of the order n, the Wiener index $W(G)$, the geometric mean of the transmission degrees sequence $M(G)$ and the parameter α. It also gives an upper bound for $D_{\alpha}E(G)$ in terms of the order n, the diameter d and the parameter α.

Theorem 4. *Assume that G is a connected graph of order $n \geq 2$ with diameter d. Then,*

$$\begin{aligned} & e^{\sqrt{\frac{4W^2(G)-M^2(G)n}{n(n-1)}} - \frac{2\alpha W(G)}{n}} + (n-1)\left(e^{\frac{2\alpha W(G)}{n}} - \left(\sqrt{\frac{4W^2(G)-M^2(G)n}{n(n-1)}}\right)\right)^{\frac{1}{n-1}} \\ & \leq D_{\alpha}E(G) \leq \\ & n-1+e^{\sqrt{n(n-1)\left((1-\alpha)^2 d^2 + \frac{\alpha^2 n^2 (n-1)}{4} - \alpha^2 (n-1)\right)}}. \end{aligned} \tag{12}$$

The equality on the left-hand side of (12) holds if and only if $G = K_n$. The equality on the right hand side of (12) holds if and only if $G = K_1$.

Proof. We will deal with the left part inequality first. Thanks to the arithmetic–geometric mean inequality, we arrive at

$$\begin{aligned} D_\alpha E(G) &= e^{\partial_1 - \frac{2\alpha W(G)}{n}} + e^{\partial_2 - \frac{2\alpha W(G)}{n}} + \cdots + e^{\partial_n - \frac{2\alpha W(G)}{n}} \\ &\geq e^{\partial_1 - \frac{2\alpha W(G)}{n}} + (n-1)\left(\prod_{i=2}^{n} e^{\partial_i - \frac{2\alpha W(G)}{n}}\right)^{\frac{1}{n-1}} \\ &= e^{\partial_1 - \frac{2\alpha W(G)}{n}} + (n-1)\left(e^{\frac{2\alpha W(G)}{n} - \partial_1}\right)^{\frac{1}{n-1}}. \end{aligned} \tag{13}$$

By Lemma 3, $\partial_1 \geq \sqrt{\frac{\sum_{i=1}^{n} Tr_i^2}{n}}$. Setting $\sqrt{a_i} = Tr_i$ in Lemma 6, we get

$$n^2\left[\frac{\sum_{i=1}^{n} Tr_i^2}{n} - \left(\frac{2W(G)}{n}\right)^2\right] \geq \sum_{i=1}^{n} Tr_i^2 - n\left(\prod_{i=1}^{n} Tr_i^2\right)^{\frac{1}{n}}.$$

Combining this with Lemma 3 yields

$$\partial_1 \geq \sqrt{\frac{4W^2(G) - M^2(G)n}{n(n-1)}}. \tag{14}$$

Clearly, $\sqrt{\frac{4W^2(G)-M^2(G)n}{n(n-1)}} \geq \frac{2W(G)}{n}$, and so

$$\sqrt{\frac{4W^2(G) - M^2(G)n}{n(n-1)}} - \frac{2\alpha W(G)}{n} \geq (1-\alpha)\frac{2W(G)}{n} \geq 0.$$

Similar to Theorem 3, we obtain the desired result. If $G = K_n$, we have $\partial_1 = n-1, \partial_2 = \cdots = \partial_n = \alpha n - 1$, $W(G) = \frac{n(n-1)}{2}$, and $M(G) = n-1$. Therefore, $D_\alpha E(G) = e^{(1-\alpha)(n-1)} + (n-1)e^{\alpha - 1}$ and the equality holds.

Conversely, assume that the equality holds true. In view of (13), we have $\partial_2 = \cdots = \partial_n$. Clearly, $4W^2(G) = M^2(G)n$ if and only if $n = 1$. From (14), it follows that $\partial_1 > 0$ for $n \geq 2$. Thus, G has exactly two distinct generalized distance eigenvalues, and so Lemma 2 implies that G is the complete graph K_n.

Next, we prove the right inequality. We have

$$
\begin{aligned}
D_\alpha E(G) &= n + \sum_{i=1}^{n} \sum_{k\geq 1} \frac{\left(\partial_i - \frac{2\alpha W(G)}{n}\right)^k}{k!} \\
&\leq n + \sum_{i=1}^{n} \sum_{k\geq 1} \frac{\left|\partial_i - \frac{2\alpha W(G)}{n}\right|^k}{k!} \\
&= n + \sum_{k\geq 1} \frac{1}{k!} \sum_{i=1}^{n} \left[\left(\partial_i - \frac{2\alpha W(G)}{n}\right)^2\right]^{\frac{k}{2}} \\
&\leq n + \sum_{k\geq 1} \frac{1}{k!} \left[\sum_{i=1}^{n} \left(\partial_i - \frac{2\alpha W(G)}{n}\right)^2\right]^{\frac{k}{2}} \\
&= n + \sum_{k\geq 1} \frac{1}{k!} \left[2(1-\alpha)^2 \sum_{1\leq i<j\leq n} d_{ij}^2 + \alpha^2 \sum_{i=1}^{n} Tr_i^2 - \frac{4\alpha^2 W^2(G)}{n}\right]^{\frac{k}{2}} \\
&= n - 1 + \sum_{k\geq 0} \frac{\left(\sqrt{2(1-\alpha)^2 \sum_{1\leq i<j\leq n} d_{ij}^2 + \alpha^2 \sum_{i=1}^{n} Tr_i^2 - \frac{4\alpha^2 W^2(G)}{n}}\right)^k}{k!} \\
&= n - 1 + e^{\sqrt{2(1-\alpha)^2 \sum_{1\leq i<j\leq n} d_{ij}^2 + \alpha^2 \sum_{i=1}^{n} Tr_i^2 - \frac{4\alpha^2 W^2(G)}{n}}}.
\end{aligned}
$$

As $d_{ij} \leq d$ for $i \neq j$ and there are $\frac{n(n-1)}{2}$ pairs of vertices in G, we have $2(1-\alpha)^2 \sum_{1\leq i<j\leq n} d_{ij}^2 + \alpha^2 \sum_{i=1}^{n} Tr_i^2 - \frac{4\alpha^2 W^2(G)}{n} \leq 2(1-\alpha)^2 \frac{n(n-1)}{2} d^2 + \frac{\alpha^2 n^3 (n-1)^2}{4} - \alpha^2 n(n-1)^2$, so that

$$
D_\alpha E(G) \leq n - 1 + e^{\sqrt{n(n-1)\left(1-\alpha)^2 d^2 + \frac{\alpha^2 n^2 (n-1)}{4} - \alpha^2 (n-1)\right)}}.
$$

Therefore, we arrive at the right-hand side of the inequality (12).

In the above proof, it can be seen that the equality holds if and only if G has no non-zero D_α-eigenvalues. Recall that G is connected. This can only happen when $G \cong K_1$. The proof is complete. □

Remark 1. *In view of the inequality* $\frac{2W(G)}{n} \geq M(G)$*, we obtain*

$$
\sqrt{\frac{4W^2(G) - M^2(G)n}{n(n-1)}} \geq \frac{2W(G)}{n}.
$$

Recall that the function $f(x)$ defined in (11) is increasing. The given lower bound in (12) turns out to be sharper than the lower bound in (8).

Given a k-transmission regular graph G, we have $W(G) = \frac{nk}{2}$ and $M(G) = k$. Therefore, the following result follows immediately from Theorem 4.

Corollary 2. *Suppose that G is k-transmission regular. We have*

$$
D_\alpha E(G) \geq e^{(1-\alpha)k} + (n-1)e^{\frac{(\alpha-1)k}{n-1}},
$$

where the equality holds if and only if $G = K_n$.

The next result provides a lower bound for $D_\alpha E(G)$ involving the order n and the Wiener index $W(G)$.

Theorem 5. *Suppose that G is a connected graph of order n. We have*

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

Proof. Applying the Cauchy–Schwartz inequality we have $\left(\sum_{i=1}^n Tr_i\right)^2 \leq n\sum_{i=1}^n Tr_i^2$, therefore

$$\sum_{i=1}^n Tr_i^2 \geq \frac{4W^2(G)}{n}. \tag{15}$$

It follows again by the Cauchy–Schwartz inequality that

$$Tr_i^2 = \left(\sum_{j=1}^n d_{ij}\right)^2 \leq n\sum_{j=1}^n d_{ij}^2.$$

Thus

$$\sum_{i=1}^n Tr_i^2 \leq n\sum_{i=1}^n\sum_{j=1}^n d_{ij}^2,$$

and then, by (15), we obtain

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

Consequently, we have

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

□

Corollary 3. *Suppose that G is connected with order n. We have*

$$D_\alpha E(G) > n + \frac{1}{2}(1-\alpha)^2(n-1)^2.$$

Proof. As $d_{ij} \geq 1$ for $i \neq j$ and there are $\frac{n(n-1)}{2}$ pairs of vertices in G, by Theorem 5, we obtain

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

and the result follows. □

4. Upper Bounds for the Generalized Distance Estrada Index of Graphs

In this section, we obtain some upper bounds for the generalized distance Estrada index $D_\alpha E(G)$ of a connected graph G involving the order n, the Wiener index $W(G)$, the transmission degrees as well as the parameter $\alpha \in [0,1]$. We also characterize the extremal graphs attaining these bounds.

The next result gives an upper bound for the generalized distance Estrada index $D_\alpha E(G)$ using the order n, the Wiener index $W(G)$, the transmission degrees as well as the parameter α.

Theorem 6. *Suppose that G is connected with order n. For any integer $k_0 \geq 2$,*

$$\begin{aligned} D_\alpha E(G) &\leq n - 1 - \sqrt{2(1-\alpha)^2 \sum_{1\leq i<j\leq n} d_{ij}^2 + \alpha^2 \sum_{i=1}^{n} Tr_i^2 - \frac{4\alpha^2 W^2(G)}{n}} \\ &+ \sum_{k=2}^{k_0} \frac{U_k(G) - \left(\sqrt{2(1-\alpha)^2 \sum_{1\leq i<j\leq n} d_{ij}^2 + \alpha^2 \sum_{i=1}^{n} Tr_i^2 - \frac{4\alpha^2 W^2(G)}{n}}\right)^k}{k!} \\ &+ e^{\sqrt{2(1-\alpha)^2 \sum_{1\leq i<j\leq n} d_{ij}^2 + \alpha^2 \sum_{i=1}^{n} Tr_i^2 - \frac{4\alpha^2 W^2(G)}{n}}}, \end{aligned} \tag{16}$$

where the equality holds if and only if $G = K_1$.

Proof. By definition of $D_\alpha E(G)$, we have

$$\begin{aligned} D_\alpha E(G) &= \sum_{k=0}^{k_0} \frac{U_k(G)}{k!} + \sum_{k\geq k_0+1} \frac{1}{k!} \sum_{i=1}^{n} \left(\partial_i - \frac{2\alpha W(G)}{n}\right)^k \\ &\leq \sum_{k=0}^{k_0} \frac{U_k(G)}{k!} + \sum_{k\geq k_0+1} \frac{1}{k!} \sum_{i=1}^{n} \left|\partial_i - \frac{2\alpha W(G)}{n}\right|^k \\ &\leq \sum_{k=0}^{k_0} \frac{U_k(G)}{k!} + \sum_{k\geq k_0+1} \frac{1}{k!} \left(\sum_{i=1}^{n} \left(\partial_i - \frac{2\alpha W(G)}{n}\right)^2\right)^{\frac{k}{2}} \\ &= \sum_{k=0}^{k_0} \frac{U_k(G)}{k!} + \sum_{k\geq k_0+1} \frac{\left(\sqrt{2(1-\alpha)^2 \sum_{1\leq i<j\leq n} d_{ij}^2 + \alpha^2 \sum_{i=1}^{n} Tr_i^2 - \frac{4\alpha^2 W^2(G)}{n}}\right)^k}{k!} \\ &= \sum_{k=0}^{k_0} \frac{U_k(G)}{k!} + e^{\sqrt{2(1-\alpha)^2 \sum_{1\leq i<j\leq n} d_{ij}^2 + \alpha^2 \sum_{i=1}^{n} Tr_i^2 - \frac{4\alpha^2 W^2(G)}{n}}} \\ &- \sum_{k=0}^{k_0} \frac{\left(\sqrt{2(1-\alpha)^2 \sum_{1\leq i<j\leq n} d_{ij}^2 + \alpha^2 \sum_{i=1}^{n} Tr_i^2 - \frac{4\alpha^2 W^2(G)}{n}}\right)^k}{k!}, \end{aligned}$$

and (16) follows. Thanks to (16), the equality is attained in (16) if and only if G has no non-zero D_α-eigenvalues, i.e., $G \cong K_1$. The proof is complete. □

Remark 2. *Notice that we have*

$$\begin{aligned} U_k(G) &= \sum_{i=1}^{n}\left(\partial_i - \frac{2\alpha W(G)}{n}\right)^k \\ &\leq \sum_{i=1}^{n}\left|\partial_i - \frac{2\alpha W(G)}{n}\right|^k \leq \left(\sum_{i=1}^{n}\left(\partial_i - \frac{2\alpha W(G)}{n}\right)^2\right)^{\frac{k}{2}} = (U_2(G))^{\frac{k}{2}}, \end{aligned}$$

where the second inequality can be derived from the following fact:

For non-negative integers $a_1, a_2, \ldots, a_n$ and integer $k \geq 2$,

$$\sum_{i=1}^{n} a_i^k \leq \left(\sum_{i=1}^{n} a_i^2\right)^{\frac{k}{2}}. \tag{17}$$

Therefore, $U_k(G) - \left(\sqrt{U_2(G)}\right)^k \leq 0$. Then,

$$\sum_{k=2}^{k_0} \frac{U_k(G) - \left(\sqrt{2(1-\alpha)^2 \sum_{1\leq i<j\leq n} d_{ij}^2 + \alpha^2 \sum_{i=1}^{n} Tr_i^2 - \frac{4\alpha^2 W^2(G)}{n}}\right)^k}{k!} \leq 0.$$

It follows from Theorem 6 that

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

Putting $\alpha = 0$, we get the following upper bound for the distance Estrada index,

$$DEE(G) = D_0E(G) \leq n - 1 - \sqrt{2\sum_{1\leq i<j\leq n} d_{ij}^2} + e^{\sqrt{2\sum_{1\leq i<j\leq n} d_{ij}^2}}. \tag{18}$$

Remark 3. *The following upper bound for the distance Estrada index $DEE(G)$ was obtained in [22]. Let G be a connected graph of order n and diameter d. Then,*

$$DEE(G) \leq n - 1 + e^{d\sqrt{n(n-1)}}. \tag{19}$$

It is easily seen that the upper bound given in (18) is better than the upper bound given in (19).

The last upper bound is as follows.

Theorem 7. *Suppose that G is connected with order n. For any integer $k_0 \geq 2$,*

$$\begin{aligned} D_\alpha E(G) &\leq n - 2 - \partial_1 + \frac{2\alpha W(G)}{n} - \sqrt{\xi} \\ &+ \sum_{k=2}^{k_0} \frac{U_k(G) - \left(\partial_1 - \frac{2\alpha W(G)}{n}\right)^k - \left(\sqrt{\xi}\right)^k}{k!} + e^{\partial_1 - \frac{2\alpha W(G)}{n}} + e^{\sqrt{\xi}}, \end{aligned} \tag{20}$$

where $\xi = 2(1-\alpha)^2 \sum_{1\le i<j\le n} d_{ij}^2 + \alpha^2 \sum_{i=1}^n Tr_i^2 - \frac{4\alpha^2 W^2(G)}{n} - \left(\partial_1 - \frac{2\alpha W(G)}{n}\right)^2$, *with equality if and only if* $G = K_1$.

Proof. Notice that

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

Using the inequality (17), we have

$$\begin{aligned}
& D_\alpha E(G) - e^{\partial_1 - \frac{2\alpha W(G)}{n}} \\
&= \sum_{k=0}^{k_0} \frac{U_k(G) - \left(\partial_1 - \frac{2\alpha W(G)}{n}\right)^k}{k!} + \sum_{k\ge k_0+1} \frac{1}{k!} \sum_{i=2}^{n}\left(\partial_i - \frac{2\alpha W(G)}{n}\right)^k \\
&\le \sum_{k=0}^{k_0} \frac{U_k(G) - \left(\partial_1 - \frac{2\alpha W(G)}{n}\right)^k}{k!} + \sum_{k\ge k_0+1} \frac{1}{k!} \sum_{i=2}^{n}\left|\partial_i - \frac{2\alpha W(G)}{n}\right|^k \\
&\le \sum_{k=0}^{k_0} \frac{U_k(G) - \left(\partial_1 - \frac{2\alpha W(G)}{n}\right)^k}{k!} + \sum_{k\ge k_0+1} \frac{1}{k!} \left(\sum_{i=2}^{n}\left(\partial_i - \frac{2\alpha W(G)}{n}\right)^2\right)^{\frac{k}{2}} \\
&= \sum_{k=0}^{k_0} \frac{U_k(G) - \left(\partial_1 - \frac{2\alpha W(G)}{n}\right)^k}{k!} \\
&+ \sum_{k\ge k_0+1} \frac{\left(\sqrt{2(1-\alpha)^2 \sum_{1\le i<j\le n} d_{ij}^2 + \alpha^2 \sum_{i=1}^n Tr_i^2 - \frac{4\alpha^2 W^2(G)}{n} - (\partial_1 - \frac{2\alpha W(G)}{n})^2}\right)^k}{k!} \\
&= \sum_{k=0}^{k_0} \frac{U_k(G) - \left(\partial_1 - \frac{2\alpha W(G)}{n}\right)^k}{k!} \\
&+ e^{\sqrt{2(1-\alpha)^2 \sum_{1\le i<j\le n} d_{ij}^2 + \alpha^2 \sum_{i=1}^n Tr_i^2 - \frac{4\alpha^2 W^2(G)}{n} - \left(\partial_1 - \frac{2\alpha W(G)}{n}\right)^2}} \\
&- \sum_{k=0}^{k_0} \frac{\left(\sqrt{2(1-\alpha)^2 \sum_{1\le i<j\le n} d_{ij}^2 + \alpha^2 \sum_{i=1}^n Tr_i^2 - \frac{4\alpha^2 W^2(G)}{n} - (\partial_1 - \frac{2\alpha W(G)}{n})^2}\right)^k}{k!},
\end{aligned}$$

where by the power-series expansion of $e^x = \sum_{k\ge 0} \frac{x^k}{k!}$, we have

$$\begin{aligned}
& e^{\sqrt{2(1-\alpha)^2 \sum_{1\le i<j\le n} d_{ij}^2 + \alpha^2 \sum_{i=1}^n Tr_i^2 - \frac{4\alpha^2 W^2(G)}{n} - \left(\partial_1 - \frac{2\alpha W(G)}{n}\right)^2}} \\
&= \sum_{k=0}^{k_0} \frac{\left(\sqrt{2(1-\alpha)^2 \sum_{1\le i<j\le n} d_{ij}^2 + \alpha^2 \sum_{i=1}^n Tr_i^2 - \frac{4\alpha^2 W^2(G)}{n} - (\partial_1 - \frac{2\alpha W(G)}{n})^2}\right)^k}{k!} \\
&+ \sum_{k\ge k_0+1} \frac{\left(\sqrt{2(1-\alpha)^2 \sum_{1\le i<j\le n} d_{ij}^2 + \alpha^2 \sum_{i=1}^n Tr_i^2 - \frac{4\alpha^2 W^2(G)}{n} - (\partial_1 - \frac{2\alpha W(G)}{n})^2}\right)^k}{k!},
\end{aligned}$$

and the last equality holds. This completes the proof. □

5. Relationship between the Generalized Distance Estrada Index and Generalized Distance Energy of Graphs

The energy $E(G)$ of a graph G, first introduced in [34], is defined as the sum of absolute values of eigenvalues of the adjacency matrix of G. Since then, $E(G)$ has found a wide range of applications in chemical mathematics and has been investigated extensively by mathematicians. In addition to adjacency matrix, the energy of Laplacian, distance Laplacian, signless Laplacian as well as distance signless Laplacian has also been studied; see works [4,32,33,35–37] and the references therein for more details. Recently, the authors of [38] considered a novel energy with respect to the generalized distance matrix of a graph. The *generalized distance energy*, denoted by $E^{D_\alpha}(G)$, is defined as

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

It is clear from the definition that $E^{D_0}(G) = E^{D}(G)$ and $2E^{D_{\frac{1}{2}}}(G) = E^{Q}(G)$, where $E^{D}(G)$ and $E^{Q}(G)$ denotes, respectively, the distance energy and the distance signless Laplacian energy of a graph G. This shows that the concept of generalized distance energy of a graph G merges the theories of distance energy and the distance signless Laplacian energy of a graph G. Therefore, it will be interesting to study the quantity $E^{D_\alpha}(G)$ and explore some properties like the bounds, the dependence on the structure of graph G, and the dependence on the parameter α and its relation with other graph-spectrum-based invariants. The authors of [38] give some bounds for $E^{D_\alpha}(G)$ and have investigated its dependence on the graph topology as well as the parameter α. Our aim in this section is to explore the relationship between generalized distance Estrada index $D_\alpha E(G)$ and generalized distance energy $E^{D_\alpha}(G)$ of a simple connected graph G.

Theorem 8. *Suppose that G is a connected graph with order n and diameter d. We have*

$$\begin{aligned} D_\alpha E(G) - E^{D_\alpha}(G) \quad &\leq \quad n - 1 - \sqrt{n(n-1)\left((1-\alpha)^2 d^2 + \frac{\alpha^2 n^2 (n-1)}{4} - \alpha^2 (n-1)\right)} \\ &+ \quad e^{\sqrt{n(n-1)\left((1-\alpha)^2 d^2 + \frac{\alpha^2 n^2 (n-1)}{4} - \alpha^2 (n-1)\right)}}, \end{aligned} \tag{21}$$

and

$$D_\alpha E(G) \leq n - 1 + e^{E^{D_\alpha}}(G). \tag{22}$$

Equality holds in (21) and (22) if and only if $G \cong K_1$.

Proof. Starting with Equation (2), we have

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

Taking into account the definition of the generalized distance energy, we obtain

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

which leads to

$$\begin{aligned} D_\alpha E(G) - E^{D_\alpha}(G) &\leq n + \sum_{i=1}^{n} \sum_{k\geq 2} \frac{\left|\partial_i - \frac{2\alpha W(G)}{n}\right|^k}{k!} \\ &\leq n - 1 - \sqrt{2(1-\alpha)^2 \sum_{1\leq i<j\leq n} d_{ij}^2 + \alpha^2 \sum_{i=1}^{n} Tr_i^2 - \frac{4\alpha^2 W^2(G)}{n}} \\ &\quad + e^{\sqrt{2(1-\alpha)^2 \sum_{1\leq i<j\leq n} d_{ij}^2 + \alpha^2 \sum_{i=1}^{n} Tr_i^2 - \frac{4\alpha^2 W^2(G)}{n}}}. \end{aligned}$$

Notice that the function $f(x) = e^x - x$ monotonically increases for $x \geq 0$. Therefore, the minimum upper bound for $D_\alpha E(G) - E^{D_\alpha}(G)$ is attained for $2(1-\alpha)^2 \sum_{1\leq i<j\leq n} d_{ij}^2 + \alpha^2 \sum_{i=1}^{n} Tr_i^2 - \frac{4\alpha^2 W^2(G)}{n} \leq 2(1-\alpha)^2 \frac{n(n-1)}{2} d^2 + \frac{\alpha^2 n^3 (n-1)^2}{4} - \alpha^2 n(n-1)^2$, and we have

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

Another way to obtain the relation between $D_\alpha E(G)$ and $E^{D_\alpha}(G)$ is as follows,

$$\begin{aligned} D_\alpha E(G) &\leq n + \sum_{i=1}^{n} \sum_{k\geq 1} \frac{\left|\partial_i - \frac{2\alpha W(G)}{n}\right|^k}{k!} \\ &\leq n + \sum_{k\geq 1} \frac{1}{k!} \left(\sum_{i=1}^{n} \left|\partial_i - \frac{2\alpha W(G)}{n}\right| \right)^k \\ &= n + \sum_{k\geq 1} \frac{\left(E^{D_\alpha}(G)\right)^k}{k!} \\ &= n - 1 + \sum_{k\geq 0} \frac{\left(E^{D_\alpha}(G)\right)^k}{k!}, \end{aligned}$$

implying

$$D_\alpha E(G) \leq n - 1 + e^{E^{D_\alpha}}(G).$$

Moreover, equality holds in (21) and (22) if and only if $G \cong K_1$. □

Theorem 9. *Assume that G is connected with order n and $0 \leq \alpha < 1$. Then,*

$$D_\alpha E(G) \leq n - 1 - E^{D_\alpha}(G) + e^{E^{D_\alpha}(G)},$$

where the equality holds if and only if $G = K_1$.

Proof. Notice that it holds $\sum_{i=1}^{n}\left(\partial_i - \frac{2\alpha W(G)}{n}\right) = 0$ and $\partial_1 \geq \frac{2W(G)}{n}$. From the definition of $D_\alpha E(G)$, we get

$$\begin{aligned} D_\alpha E(G) &= \sum_{i=1}^{n} e^{\left(\partial_i - \frac{2\alpha W(G)}{n}\right)} = n + \sum_{k\geq 2} \frac{1}{k!} \sum_{i=1}^{n} \left(\partial_i - \frac{2\alpha W(G)}{n}\right)^k \\ &\leq n + \sum_{k\geq 2} \frac{1}{k!} \left(\sum_{i=1}^{n} \left|\partial_i - \frac{2\alpha W(G)}{n}\right|\right)^k = n + \sum_{k\geq 2} \frac{1}{k!} \left(E^{D_\alpha}(G)\right)^k \\ &= n - 1 - E^{D_\alpha}(G) + e^{E^{D_\alpha}(G)}, \end{aligned}$$

with equality attained if and only if $\sum_{i=1}^{n}\left(\partial_i - \frac{2\alpha W(G)}{n}\right)^k = \left(\sum_{i=1}^{n}\left|\partial_i - \frac{2\alpha W(G)}{n}\right|\right)^k$ holds for all integers $k \geq 2$, i.e., if and only if at most one of $\partial_i - \frac{2\alpha W(G)}{n}$ for $i = 1, 2, \ldots, n$ is positive and all others are equal to zero, i.e., $\partial_2 = \cdots = \partial_n = \frac{2\alpha W(G)}{n}$. As $\sum_{i=1}^{n} \partial_i = 2\alpha W(G)$, then $\partial_1 = \frac{2\alpha W(G)}{n}$, which is in contradiction with $\partial_1 \geq \frac{2W(G)}{n}$. Therefore $G = K_1$, and the proof is complete. □

Remark 4. *The following upper bound for the distance Estrada index $DEE(G)$ was obtained in [22],*

$$DEE(G) \leq n - 1 + e^{E^D(G)}. \tag{23}$$

Putting $\alpha = 0$ in the upper bound of Theorem 9, we can easily see that the resulting upper bound for the distance Estrada index is better than the upper bound given by (23).

Theorem 10. *Assume that G is connected with order n. We have*

$$\frac{1}{2}E^{D_\alpha}(G)(e-1) + n - t \leq D_\alpha E(G) \leq n - 1 + e^{\frac{E^{D_\alpha}(G)}{2}}, \tag{24}$$

where t means the number of eigenvalues with $\partial_t > \frac{2\alpha W(G)}{n}$. Furthermore, the equality holds on both sides of (24) if and only if $G = K_1$.

Proof. We will first prove the left inequality. Suppose that t is an integer such that $\partial_t > \frac{2\alpha W(G)}{n}$ and $\partial_{t+1} \leq \frac{2\alpha W(G)}{n}$. As $e^x \geq ex$, equality holds if and only if $x = 1$ and $e^x \geq 1 + x$, equality holds if and only if $x = 0$. We have

$$\begin{aligned} D_\alpha E(G) &= \sum_{i=1}^{n} e^{\left(\partial_i - \frac{2\alpha W(G)}{n}\right)} = \sum_{i=1}^{t} e^{\left(\partial_i - \frac{2\alpha W(G)}{n}\right)} + \sum_{i=t+1}^{n} e^{\left(\partial_i - \frac{2\alpha W(G)}{n}\right)} \\ &\geq \sum_{i=1}^{t} e\left(\partial_i - \frac{2\alpha W(G)}{n}\right) + \sum_{i=t+1}^{n}\left(1 + \partial_i - \frac{2\alpha W(G)}{n}\right) \\ &= e\left(\partial_1 + \partial_2 + \cdots + \partial_t - \frac{2\alpha t W(G)}{n}\right) + (n-t) + \left(\partial_{t+1} + \cdots + \partial_n - \frac{2\alpha(n-t)W(G)}{n}\right) \\ &= (e-1)\left(\partial_1 + \partial_2 + \cdots + \partial_t - \frac{2\alpha t W(G)}{n}\right) + (n-t) + \sum_{i=1}^{n}\left(\partial_i - \frac{2\alpha W(G)}{n}\right) \\ &= \frac{1}{2}E^{D_\alpha}(G)(e-1) + n - t. \end{aligned}$$

Next, we want to prove the right inequality. Since $f(x) = e^x$ monotonically increases in the interval $(-\infty, \infty)$, we obtain

$$\begin{aligned}
D_\alpha E(G) &= \sum_{i=1}^{n} e^{\partial_i - \frac{2\alpha W(G)}{n}} \le n - t + \sum_{i=1}^{t} e^{\partial_i - \frac{2\alpha W(G)}{n}} \\
&= n - t + \sum_{i=1}^{t} \sum_{k\ge 0} \frac{\left(\partial_i - \frac{2\alpha W(G)}{n}\right)^k}{k!} \\
&= n + \sum_{k\ge 1} \frac{1}{k!} \sum_{i=1}^{t} \left(\partial_i - \frac{2\alpha W(G)}{n}\right)^k \\
&\le n + \sum_{k\ge 1} \frac{1}{k!} \left(\sum_{i=1}^{t} \left(\partial_i - \frac{2\alpha W(G)}{n}\right)\right)^k \\
&= n - 1 + e^{\frac{E^{D_\alpha}(G)}{2}}.
\end{aligned}$$

We observe that the equality holds on both sides of (24) if and only if $E^{D_\alpha}(G) = 0$. This only happens when $G = K_1$ since G is a connected graph. □

Remark 5. *We observe that the upper bound given in (24) is better than the upper bound given in (22). Also, putting $\alpha = 0$ in the upper bound of Theorem 10, we can easily see that the resulting upper bound for the distance Estrada index is also better than the upper bound given by (23).*

6. Examples

In this section, we obtain some results about the generalized distance Estrada index of some typical graphs. This would be instrumental in interpreting this measure further in the case of more complex graphs. We also give an expression for $D_\alpha E(G)$ of a (transmission) regular graph G, in terms of the distance eigenvalues as well as adjacency eigenvalues of G, and describe the generalized distance Estrada index of some graphs obtained by operations.

As mentioned in introduction of the paper, for $\alpha = 0$ the generalized distance matrix $D_\alpha(G)$ is equivalent to the distance matrix $D(G)$ and for $\alpha = \frac{1}{2}$, twice the generalized distance matrix $D_\alpha(G)$ is the same as the distance signless Laplacian matrix $D^Q(G)$. Therefore, if in particular we put $\alpha = 0$ and $\alpha = \frac{1}{2}$ in all the results obtained in this paper, we obtain the corresponding bounds for the distance Estrada index $DEE(G)$ and the distance signless Laplacian Estrada index $D_E^Q E(G)$, respectively.

Theorem 11. *Suppose that G is a k-transmission regular graph of order n having distance eigenvalues $\mu_1, \mu_2, \ldots, \mu_n$. Then,*

$$D_\alpha E(G) = \sum_{i=1}^{n} e^{(1-\alpha)\mu_i}.$$

Proof. Note that the generalized distance spectrum of the graph G consists of $\alpha k + (1-\alpha)\mu_1 \ge \alpha k + (1-\alpha)\mu_2 \ge \cdots \ge \alpha k + (1-\alpha)\mu_n$, where $\mu_1 \ge \cdots \ge \mu_n$ is the distance spectrum of G. Also, it is easy to see that $W(G) = \frac{nk}{2}$. Then, $D_\alpha E(G) = \sum_{i=1}^{n} e^{\alpha k + (1-\alpha)\mu_i - \alpha k} = DEE(G) = \sum_{i=1}^{n} e^{(1-\alpha)\mu_i}$. □

Theorem 12. *Let G be an r-regular graph of order n, size m and diameter at most 2. If $\{r, \lambda_2, \ldots, \lambda_n\}$ are the eigenvalues of the adjacency matrix $A(G)$ of G, then*

$$D_\alpha E(G) = e^{n(2n-r-2)-2\alpha(n^2-n-m)} + \sum_{i=2}^{n} e^{\alpha(n\lambda_i+rn+2n+2m)-n(\lambda_i+2)}.$$

Proof. The transmission of each vertex $v \in V(G)$ can be computed as $Tr(v) = d(v) + 2(n - d(v) - 1) = 2n - d(v) - 2$ and the Wiener index $W(G)$ of G becomes $W(G) = n^2 - n - m$. Also,

$$\begin{aligned} D_\alpha(G) = \alpha Tr(G) + (1-\alpha)D(G) &= \alpha(2n-r-2)I + (1-\alpha)(2J - 2I - A(G)) \\ &= \alpha((2n-r-2)I - 2J + 2I + A(G)) + 2J - 2I - A(G), \end{aligned}$$

where J is the all ones matrix. Then,

$$\begin{aligned} D_\alpha E(G) &= \sum_{i=1}^{n} e^{\partial_i - \frac{2\alpha W(G)}{n}} = e^{(2n-r-2)-\frac{2\alpha(n^2-n-m)}{n}} + \sum_{i=2}^{n} e^{(\alpha(2n+\lambda_i-r)-\lambda_i-2)-\frac{2\alpha(n^2-n-m)}{n}} \\ &= e^{n(2n-r-2)-2\alpha(n^2-n-m)} + \sum_{i=2}^{n} e^{\alpha(n\lambda_i+rn+2n+2m)-n(\lambda_i+2)}. \end{aligned}$$

□

We denote by $G \times H$ the *cartesian product* of two graphs G and H. It is the graph with vertex set $V(G) \times V(H)$ and two vertices (u_1, u_2) and (v_1, v_2) are adjacent if and only if $u_1 = v_1$ and $u_2v_2 \in E(H)$ or $u_2 = v_2$ and $u_1v_1 \in E(G)$.

Corollary 4. *Let G be an r-regular graph of diameter at most 2 with an adjacency matrix A and $spec(G) = \{r, \lambda_2, \ldots, \lambda_n\}$. Then, the generalized distance Estrada index of $H = G \times K_2$ is*

$$D_\alpha E(H) = n - 1 + e^{(1-\alpha)(5n-2r-4)} + e^{(\alpha-1)n} + \sum_{i=2}^{n} e^{(\alpha-1)(2\lambda_i+4)}.$$

Proof. Let $V(G) = \{v_1, v_2, \ldots, v_n\}$, $V(K_2) = \{w_1, w_2\}$. As $d_H((v_i, w_j), (v_s, w_t)) = d_G(v_i, v_s) + d_{K_2}(w_j, w_t) = d_G(v_i, v_s) + 1$, we see that all vertices of H have the same transmission and $Tr_H(v_i, w_j) = 5n - 2r - 4$. So $Tr(H) = (5n - 2r - 4)I$. Then $W(H) = \frac{n(5n-2r-4)}{2}$. Note that $H = G \times K_2$ has distance spectrum (see in [37]) $spec(H) = \left\{5n - 2(r+2), -2(\lambda_i + 2), -n, 0^{[n-1]}\right\}$, for $i = 2, \ldots, n$.

Then,

$$D_\alpha E(H) = n - 1 + e^{(1-\alpha)(5n-2r-4)} + e^{(\alpha-1)n} + \sum_{i=2}^{n} e^{(\alpha-1)(2\lambda_i+4)}.$$

□

The graph $G\nabla G$ is obtained by joining each vertex of G to each vertex of a second copy of G.

Corollary 5. *Let G be an r-regular graph with an adjacency matrix A and $spec(G) = \{r, \lambda_2, \ldots, \lambda_n\}$. Then, the generalized distance Estrada index of $G\nabla G$ is*

$$D_\alpha E(G\nabla G) = e^{(1-\alpha)(3n-r-2)} + e^{(1-\alpha)(n-r-2)} + 2\sum_{i=2}^{n} e^{(\alpha-1)(2\lambda_i+4)}.$$

Proof. For $v \in G\nabla G$, it is easy to see that $Tr(v) = d(v) + 2(n - d(v) - 1) + n = 3n - d(v) - 2 = 3n - r - 2$. Then, $G\nabla G$ is a transmission regular graph and $Tr(G\nabla G) = (3n - r - 2)I$. Note that the $G\nabla G$ has distance spectrum (see in [37]) $spec(G\nabla G) = \left\{3n - r - 2, n - r - 2, -2(\lambda_i + 2)^{[2]}\right\}$, for $i = 2, \ldots, n$. Then,

$$D_\alpha E(G\nabla G) = e^{(1-\alpha)(3n-r-2)} + e^{(1-\alpha)(n-r-2)} + 2\sum_{i=2}^{n} e^{(\alpha-1)(2\lambda_i+4)}.$$

□

Next, we study the generalized distance Estrada index of the lexicographic product $G[H]$ of two graphs G and H. The lexicographic product of G and H can be defined as follows.

Definition 1 ([39])**.** Let G and H be two graphs on vertex sets $V(G) = \{u_1, u_2, \ldots, u_p\}$ and $V(H) = \{v_1, v_2, \ldots, v_n\}$, respectively. Their *lexicographic product* $G[H]$ is a graph defined by $V(G[H]) = V(G) \times V(H)$, the cartesian product of $V(G)$, and $V(H)$, where $u = (u_1, v_1)$ is adjacent to $v = (u_2, v_2)$ if and only if either
(a) u_1 is adjacent to v_1 in G, or
(b) $u_1 = v_1$ and u_2 is adjacent to v_2 in G.

Theorem 13. *Given a k-transmission regular graph G of order p. If H is an r-regular graph of order n with adjacency eigenvalues* $\{r, \lambda_2, \ldots, \lambda_n\}$*, then*

$$D_\alpha E(G[H]) = e^{(1-\alpha)(2n-r-2)} \sum_{i=1}^{p} e^{(1-\alpha)n\mu_i} + ne^{4(\alpha-1)} \sum_{j=2}^{n} e^{2\lambda_j(\alpha-1)},$$

where $\{\mu_1, \ldots, \mu_p\}$ *are the eigenvalues of the distance matrix* $D(G)$*.*

Proof. For $v \in G[H]$, it is easy to see that $Tr(v) = r + 2(n - r - 1) + kn = kn + 2n - r - 2$. Then $G[H]$ is a transmission regular graph and $Tr(G[H]) = (kn + 2n - r - 2)I$. Note that $G[H]$ has distance spectrum (see [40]) $spec(G[H]) = \left\{n\mu_i + 2n - r - 2, -2(\lambda_j + 2)^{[n]}\right\}$, for $i = 1, \ldots, p$ and $j = 2, \ldots, n$. Then,

$$D_\alpha E(G[H]) = e^{(1-\alpha)(2n-r-2)} \sum_{i=1}^{p} e^{(1-\alpha)n\mu_i} + ne^{4(\alpha-1)} \sum_{j=2}^{n} e^{2\lambda_j(\alpha-1)}.$$

□

Example 1. *Let C_n be a cycle of order n and K_2 be the complete graph of order 2. Then, the closed fence graph is defined as $G = C_n[K_2]$, and depicted in Figure 1. Applying Theorem 13, we will be able to compute the generalized distance Estrada index of closed fence $G = C_n[K_2]$. It is well known ([41], Theorem 3) that C_n is a k-transmission regular graph, with $k = \lfloor \frac{n^2}{4} \rfloor$. It is also clear tht the adjacency spectrum of the graph K_2 is $spec(K_2) = \{1, -1\}$. Then, applying Theorem 13, the generalized distance Estrada index of closed fence $C_n[K_2]$, according to the parity of n, is as follows.*

If $n = 2z$ (i.e., n is even), then following [2] the distance spectrum of C_n is

$$spec(C_n) = \left\{0^{[z-1]}, \frac{n^2}{4}, -\csc^2\left(\frac{\pi(2j-1)}{n}\right)\right\} \quad \textit{for} \quad j = 1, \ldots, z.$$

Thus, applying Theorem 13 we have

$$D_\alpha E(C_n[K_2]) = e^{1-\alpha}\left(z - 1 + e^{(1-\alpha)\frac{n^2}{2}} + \sum_{j=1}^{z} e^{2(\alpha-1)\csc^2\left(\frac{\pi(2j-1)}{n}\right)}\right) + 2e^{2(\alpha-1)}.$$

If $n = 2z+1$ (i.e., n is odd), then following [2] the distance spectrum of C_n is

$$spec(C_n) = \left\{\frac{n^2-1}{4}, -\frac{1}{4}\sec^2\left(\frac{\pi j}{n}\right), -\frac{1}{4}\csc^2\left(\frac{\pi(2j-1)}{2n}\right)\right\} \quad for \quad j = 1, \ldots, z.$$

Thus, applying Theorem 13 we have

$$D_\alpha E(C_n[K_2]) = e^{1-\alpha}\left(e^{(1-\alpha)\frac{n^2-1}{2}} + \sum_{j=1}^{z} e^{\frac{1}{2}(\alpha-1)\sec^2\left(\frac{\pi j}{n}\right)} + \sum_{j=1}^{z} e^{\frac{1}{2}(\alpha-1)\csc^2\left(\frac{\pi(2j-1)}{2n}\right)}\right) + 2e^{2(\alpha-1)}.$$

Figure 2 shows $D_\alpha E(C_n[K_2])$ versus n for different values of α.

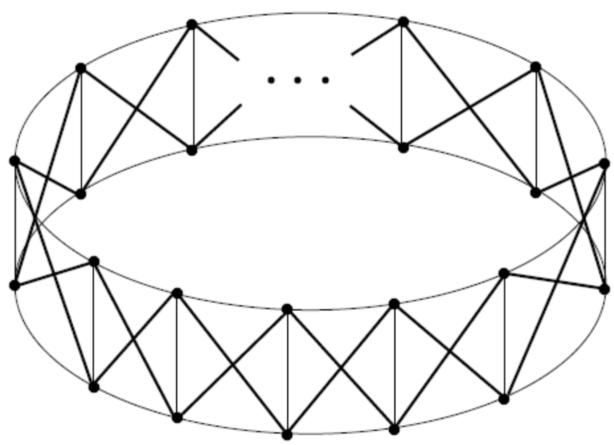

Figure 1. The closed fence graph.

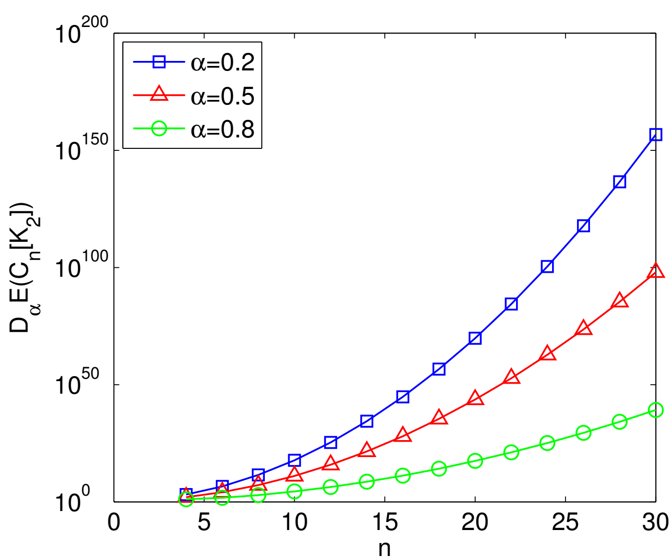

Figure 2. $D_\alpha E(C_n[K_2])$ versus n for different values of α.

7. Conclusions

The concept of Estrada index of a graph was first motivated by Ernesto Estrada in [9] as the sum of the exponential of the eigenvalues of adjacency matrix assigned to graphs. In recent years, because of the apparent success of the graph Estrada index, many variations of Estrada index have been proposed and varied Estrada indices based on the eigenvalues of other graph matrices have, one-by-one, been introduced: Estrada index-based invariant with respect to distance matrix, Laplacian matrix, signless Laplacian matrix, distance Laplacian matrix and also distance signless Laplacian matrix, etc.

As the distance and distance signless Laplacian matrices of graphs play an essential role in mathematics and are more informative than ordinary adjacency matrix, in this paper, the Estrada index of generalized distance matrix is firstly defined and investigated. In fact, this is a natural generalization of distance Estrada and distance signless Laplacian Estrada indices. Thus all properties about them can be handled by this new index, and any result regarding the spectral properties of generalized distance Estrada index, has its counterpart for each of these particular indices, and these counterparts follow immediately from a single proof. As characterization of $D_\alpha E(G)$ turns out to be highly desirable in mathematics as well as engineering, it is interesting to study the quantity $D_\alpha E(G)$ and explore some properties including the bounds, the dependence on the structure of graph G, and the dependence on the parameter α. We established some bounds for the generalized distance Estrada index $D_\alpha E(G)$ of a connected graph G, in terms of the different graph parameters including the order n, the Wiener index $W(G)$, the transmission degree, and the parameter $\alpha \in [0,1]$. We have also characterized the extremal graphs attaining these bounds. We worked out some expressions for $D_\alpha E(G)$ of some special classes of graphs.

Author Contributions: Conceptualization, A.A. and M.B.; formal analysis, A.A., M.B. and Y.S.; writing–original draft preparation, A.A and M.B.; writing–review and editing, A.A., M.B. and Y.S.; project administration, A.A.; funding acquisition, A.A. and Y.S.

Funding: The research of A. Alhevaz was in part supported by a grant from Shahrood University of Technology. Y. Shang was supported by UoA Flexible Fund No. 201920A1001 from Northumbria University.

Acknowledgments: The authors would like to thank the academic editor and the three anonymous referees for their detailed constructive comments that helped improve the quality of the paper.

Conflicts of Interest: The authors declare no conflicts of interest.

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