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On Generalized Distance Gaussian Estrada Index of Graphs

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Abstract: For a simple undirected connected graph G of order n, let $D(G)$, $D^L(G)$, $D^Q(G)$ and $Tr(G)$ be, respectively, the distance matrix, the distance Laplacian matrix, the distance signless Laplacian matrix and the diagonal matrix of the vertex transmissions of G. The generalized distance matrix $D_\alpha(G)$ is signified by $D_\alpha(G) = \alpha Tr(G) + (1-\alpha)D(G)$, where $\alpha \in [0,1]$. Here, we propose a new kind of Estrada index based on the Gaussianization of the generalized distance matrix of a graph. Let $\partial_1, \partial_2, \ldots, \partial_n$ be the generalized distance eigenvalues of a graph G. We define the generalized distance Gaussian Estrada index $P_\alpha(G)$, as $P_\alpha(G) = \sum_{i=1}^{n} e^{-\partial_i^2}$. Since characterization of $P_\alpha(G)$ is very appealing in quantum information theory, it is interesting to study the quantity $P_\alpha(G)$ and explore some properties like the bounds, the dependence on the graph topology G and the dependence on the parameter α. In this paper, we establish some bounds for the generalized distance Gaussian Estrada index $P_\alpha(G)$ of a connected graph G, involving the different graph parameters, including the order n, the Wiener index $W(G)$, the transmission degrees and the parameter $\alpha \in [0,1]$, and characterize the extremal graphs attaining these bounds.

Keywords: Gaussian Estrada index; generalized distance matrix (spectrum); Wiener index; generalized distance Gaussian Estrada index; transmission regular graph

1. Introduction

In this paper, we study connected simple graphs with a finite number of vertices. Standard graph terminology will be adopted. We refer the reader to, e.g., [1] for more related concepts. A graph is denoted by $G = (V(G), E(G))$, where $V(G) = \{v_1, v_2, \ldots, v_n\}$ is its vertex set and $E(G)$ is its edge set. The order of G is the number $n = |V(G)|$ and its size is the number $m = |E(G)|$. The set of vertices adjacent to $v \in V(G)$, denoted by $N(v)$, refers to the neighborhood of v. The degree of v, denoted by $d_G(v)$ (we simply write d_v if it is clear from the context) means the cardinality of $N(v)$. A graph is called regular if each of its vertices have the same degree. The distance between two vertices $u, v \in V(G)$, denoted by d_{uv}, is defined as the length of the shortest path between u and v in G. The diameter of G is defined as the maximum distance between any two vertices in G. The distance matrix of G is denoted by $D(G)$ and is defined as $D(G) = (d_{uv})_{u,v \in V(G)}$. The transmission $Tr_G(v)$ of a vertex v is defined as the sum of the distances from v to all other vertices in G, that is, $Tr_G(v) = \sum\limits_{u \in V(G)} d_{uv}$. A graph G

is said to be k-transmission regular if $Tr_G(v) = k$, for each $v \in V(G)$. The transmission (sometimes referred to as the Wiener index) of a graph G is denoted by $W(G)$. $W(G)$ is given by the distance sum between each pair of vertices in G. Namely, we have $W(G) = \frac{1}{2} \sum_{v \in V(G)} Tr_G(v)$. For any vertex $v_i \in V(G)$, the transmission $Tr_G(v_i)$ is also called the transmission degree, denoted by Tr_i for short and the sequence $\{Tr_1, Tr_2, \ldots, Tr_n\}$ is called the transmission degree sequence of the graph G. The second transmission degree of v_i, denoted by T_i is given by $T_i = \sum_{j=1}^{n} d_{ij} Tr_j$.

Let $Tr(G) = diag(Tr_1, Tr_2, \ldots, Tr_n)$ be the diagonal matrix of vertex transmissions of G. In [2], M. Aouchiche and P. Hansen introduced the distance Laplacian matrix $D^L(G)$ and the distance signless Laplacian matrix $D^Q(G)$ as $D^L(G) = Tr(G) - D(G)$ and $D^Q(G) = Tr(G) + D(G)$. The spectral properties of $D(G)$, $D^L(G)$ and $D^Q(G)$ have attracted much attention of researchers and a large number of papers have been published regarding their spectral properties, including spectral radius, second largest eigenvalue, smallest eigenvalue, etc. For some recent works we refer to [3–5] and the references therein.

Nikiforov [6] investigated the integration of adjacency spectrum and signless Laplacian spectrum via cunning convex combinations between diagonal degree and adjacency matrices. Recently in [7], Cui et al. introduced the generalized distance matrix $D_\alpha(G)$ as convex combinations of $Tr(G)$ and $D(G)$, defined as $D_\alpha(G) = \alpha Tr(G) + (1-\alpha)D(G)$, for $0 \le \alpha \le 1$. Since $D_0(G) = D(G)$, $2D_{\frac{1}{2}}(G) = D^Q(G)$, $D_1(G) = Tr(G)$ and $D_\alpha(G) - D_\beta(G) = (\alpha - \beta)D^L(G)$, any result regarding the spectral properties of generalized distance matrix has its counterpart for each of these particular graph matrices, and these counterparts follow immediately from a straightforward proof. In fact, this matrix leads to merging the distance spectral, distance Laplacian spectral and distance signless Laplacian spectral theories. As $D_\alpha(G)$ is a real symmetric matrix, the eigenvalues become real. Therefore, we arrange them as $\partial_1 \ge \partial_2 \ge \cdots \ge \partial_n$. The largest eigenvalue ∂_1 of the matrix $D_\alpha(G)$ is called the generalized distance spectral radius of G. For simplicity, we will refer to $\partial_1(G)$ as $\partial(G)$ in the sequel. It follows from the Perron-Frobenius theorem and the non-negativity and irreducibility of $D_\alpha(G)$ that $\partial(G)$ is the unique eigenvalue and there is a unique positive unit eigenvector X corresponding to $\partial(G)$, which is called the generalized distance Perron vector of G. As usual, K_n, $K_{s,t}$, P_n and C_n denote, respectively, the complete graph on n vertices, the complete bipartite graph on $s+t$ vertices, the path on n vertices and the cycle on n vertices.

2. Motivation

Graph spectral theory has gained momentum during the last few decades partly due to the mounting availability of scientific data and network representation stemming from a wide range of areas including biology, economics, engineering and social sciences [8]. Graph spectral techniques are proved to be highly instrumental in dissecting interconnection network structures.

Based upon investigations on geometric properties of biomolecules, Ernesto Estrada [9] considered an expression of the form

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

where $\lambda_1, \lambda_2, \ldots, \lambda_n$ are the eigenvalues of the adjacency matrix of a molecular graph G. The mathematical significance of this quantity was recognized later [10] and soon it became known under the name "Estrada index" [11]. The mathematical properties of the Estrada index have been intensively studied, see for example, [11,12]. Estrada index and its bounds have been extensively studied in the graph spectral community. We refer the interested reader to consult the recent nice survey [13].

This graph spectrum based invariant has also an important role in chemistry and physics. It can be used, for example, as a metric for the degree of folding of long chain polymeric molecules [14,15]. It has found a number of applications in complex networks and characterizes the centrality [9,16,17]. We refer the reader to [18] for an account of the numerous applications of the Estrada index.

Other than the adjacency spectrum, the Estrada index has been explored in various forms based on non-adjacency matrices in the pioneering work [9]. Because of the remarkable usefulness of the graph Estrada index, this proposal has been put into effect and varied Estrada indices based on the eigenvalues of other graph matrices have been tackled: Estrada index based invariant with respect to distance matrix, Laplacian matrix, signless Laplacian matrix, distance Laplacian matrix and distance signless Laplacian matrix, to name just a few. For some related results on this subject, see, for example, [19–23] and the references therein. Let $\mu_1, \mu_2, \ldots, \mu_n$ be the eigenvalues of the distance matrix of a graph G. Then the distance Estrada index of a connected graph G has been introduced in [20] as $DEE(G) = \sum_{i=1}^{n} e^{\mu_i}$.

A different way to study graph spectra consists of analyzing matrix functions of the matrices associated with a graph or network. In analyzing graph invariants such as centrality and communicability, matrix functions of the form $f(A) = \sum_{k=0}^{\infty} c_k A^k$ have been found as a power tool [24]. When the gap $\lambda_1 - \lambda_2$ is large, EE tends to be dominated by the largest eigenvalue λ_1. In this sense, information that is hidden in the smaller eigenvalues, which are particularly useful, for example, in the context of molecular orbital theory [25], has been overlooked. Estrada et al. [26] recently proposed to scope this bit of information by using a Gaussian matrix function, which gives rise to the Gaussian Estrada index, $H(G)$. $H(G)$ can be defined as

$$H = H(G) = trace(e^{-A^2}) = \sum_{i=1}^{n} e^{-\lambda_i^2}.$$

Gaussian Estrada index H is able to describe the partition function of quantum mechanics systems with Hamiltonian A^2 [27]. It gives more weight to eigenvalues close to zero and ideally complements the Estrada index. Moreover, it is also related to the time-dependent Schrödinger equation with the squared Hamiltonian. Based on numerical simulations, H is found to be effective in differentiating the dynamics of particle hopping among bipartite and non-bipartite structures [24]. More results can be found in [28].

A distance matrix, on the other hand, is an important variation of an adjacency matrix. It encodes information that is related to random walk and self-avoiding walks of chemical graphs which are not manifest in an adjacency matrix. Distance spectrum has been intensively tackled in the past few years [29]. In the pedigree of distance matrix, important members include distance Laplacian and distance signless Laplacian matrices.

In this work, we propose here a new kind of Estrada index based on the Gaussianization of the generalized distance matrix of a graph. The generalized distance eigenvalues of a graph G are denoted by $\partial_1, \partial_2, \ldots, \partial_n$. We define the generalized distance Gaussian Estrada index $P_\alpha(G)$, as

$$P_\alpha(G) = \sum_{i=1}^{n} e^{-\partial_i^2}. \quad (1)$$

The results for the Gaussian Estrada index of distance matrix (namely, distance Gaussian Estrada index $P^D(G)$) and Gaussian Estrada index of distance signless Laplacian matrix (namely, distance signless Laplacian Gaussian Estrada index $P^Q(G)$) can be naturally defined when setting, respectively, $\alpha = 0$ and $\alpha = \frac{1}{2}$ in the above definition.

Since characterization of $P_\alpha(G)$ tends to be very appealing in quantum information theory, it will be desirable to consider the quantity $P_\alpha(G)$ and explore some properties such as the bounds, the dependence on the structure of graph G and the dependence on the parameter α. In this paper, we aim to establish some bounds for the generalized distance Gaussian Estrada index $P_\alpha(G)$ of a connected graph G, in terms of the different graph parameters like the order n, the Wiener index $W(G)$, the transmission degrees and the parameter $\alpha \in [0,1]$. We also characterize the extremal graphs attaining these bounds. Moreover, $P_\alpha(G)$ for some fundamental special graphs has been obtained, which helps us to interpret this metric when applied to sophisticated topologies. We also give an expression for $P_\alpha(G)$ of a (transmission) regular graph G in terms of the distance eigenvalues as well as adjacency eigenvalues of G, and describe the generalized distance Gaussian Estrada index of some graphs obtained by operations.

3. Bounds for Generalized Distance Gaussian Estrada Index

We present some useful bounds in this section for the generalized distance Gaussian Estrada index $P_\alpha(G)$ of a connected graph G, in terms of the different graph parameters including the order n, the Wiener index $W(G)$, the transmission degrees and the parameter $\alpha \in [0,1]$. We will also identify the extremal graphs attaining these bounds.

We start by giving some previously known results that will be needed below.

Lemma 1. [7] *For a connected graph G of order n, we have*

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

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

Lemma 2. [7] *Define the transmission degree sequence and the second transmission degree sequence of G as $\{Tr_1, Tr_2, \ldots, Tr_n\}$ and $\{T_1, T_2, \ldots, T_n\}$, respectively. We have*

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

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

The proof of the following lemma is similar to that of Lemma 2 in [30], and is omitted here.

Lemma 3. *A connected graph G has exactly two distinct generalized distance eigenvalues if and only if G is a complete graph.*

Lemma 4. *If the transmission degree sequence of G is $\{Tr_1, Tr_2, \ldots, Tr_n\}$, then*

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

with equality if and only if G is transmission regular.

Proof. The proof is analogous to that of Theorem 2.2 in [4], and is excluded. □

Lemma 5. [31] *If A is an $n \times n$ non-negative matrix with the spectral radius $\lambda(A)$ and row sums $r_1, r_2, \dots, r_n$, then*

$$\min_{1\le i\le n} r_i \le \lambda(A) \le \max_{1\le i\le n} r_i.$$

Moreover, if A is irreducible, then both of the equalities hold if and only if the row sums of A are all equal.

Note that the i-th row sum of $D_\alpha(G)$ is $r_i = \alpha Tr_i + (1-\alpha)\sum_{j=1}^{n} d_{ij} = Tr_i$. Hence, applying Lemma 5, we derive the following result.

Corollary 1. *Let G be a simple connected graph of order n. Let $Tr_{\max}$ and $Tr_{\min}$ denote, respectively, the largest and least transmissions of G. Then $Tr_{\min} \le \partial(G) \le Tr_{\max}$. Moreover, any of the equalities holds if and only if G is a transmission regular graph.*

Next, we present the upper bounds for the generalized distance Gaussian Estrada index involving different graph invariants. To fix notation, we first introduce some preliminaries. For $k \ge 0$, define $S_k = S_k(G) = \sum_{i=1}^{n}\left(-\partial_i^2\right)^k$. Then $S_0 = n$ and $S_1 = -2(1-\alpha)^2\sum_{1\le i<j\le n}(d_{ij})^2 - \alpha^2\sum_{i=1}^{n} Tr_i^2$. A bit of basic algebra leads to the following expression:

$$P_\alpha(G) = \sum_{k\ge 0}\frac{S_k}{k!}. \tag{2}$$

Our first result gives an upper bound for the generalized distance Gaussian Estrada index $P_\alpha(G)$, through the order n the transmission degrees and the parameter α.

Theorem 1. *Let G be a connected graph of order n. Then for any integer $k_0 \ge 2$,*

$$\begin{aligned} P_\alpha(G) \;\le\;& n-1-2\left(2(1-\alpha)^2\sum_{1\le i<j\le n} d_{ij}^2 + \alpha^2\sum_{i=1}^{n} Tr_i^2\right) + e^{2(1-\alpha)^2\sum_{1\le i<j\le n} d_{ij}^2 + \alpha^2\sum_{i=1}^{n} Tr_i^2} \\ &+ \sum_{k=2}^{k_0}\frac{S_k(G) - \left(2(1-\alpha)^2\sum_{1\le i<j\le n} d_{ij}^2 + \alpha^2\sum_{i=1}^{n} Tr_i^2\right)^k}{k!}, \end{aligned} \tag{3}$$

with equality if and only if $G = K_1$.

Proof. Starting with Equation (2), we have

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

and Equation (3) follows. From the derivation of Equation (3), it is clear that the equality will be attained in Equation (3) if and only if G has no non-zero D_α-eigenvalues, i.e., $G = K_1$. □

The next result gives another upper bound as well as a lower bound for $P_\alpha(G)$ of a connected graph G.

Theorem 2. *Suppose that G is a connected graph of order n. Then for any integer $k_0 \geq 2$,*

$$
\begin{aligned}
& n - 2(1-\alpha)^2 \sum_{1\leq i<j\leq n} (d_{ij})^2 - \alpha^2 \sum_{i=1}^{n} Tr_i^2 \\
& \leq P_\alpha(G) \leq \\
& n - 2 - 2\eta + 2\partial_1^2 + \sum_{k=2}^{k_0} \frac{S_k(G) - \left(-\partial_1^2\right)^k - \xi^k}{k!} + e^{-\partial_1^2} + e^{\xi},
\end{aligned}
\tag{4}
$$

where $\xi = \eta - \partial_1^2$, and $\eta = 2(1-\alpha)^2 \sum_{1\leq i<j\leq n} d_{ij}^2 + \alpha^2 \sum_{i=1}^{n} Tr_i^2$. Equality holds on both sides of Equation (4) if and only if $G = K_1$.

Proof. We will first prove the right inequality. According to the definition of $P_\alpha(G)$, we have

$$
\begin{aligned}
P_\alpha(G) - e^{-\partial_1^2} &= \sum_{k=0}^{k_0} \frac{S_k(G) - \left(-\partial_1^2\right)^k}{k!} + \sum_{k\geq k_0+1} \frac{1}{k!} \sum_{i=2}^{n} \left(-\partial_i^2\right)^k \\
&\leq \sum_{k=0}^{k_0} \frac{S_k(G) - \left(-\partial_1^2\right)^k}{k!} + \sum_{k\geq k_0+1} \frac{1}{k!} \sum_{i=2}^{n} \left|-\partial_i^2\right|^k \\
&\leq \sum_{k=0}^{k_0} \frac{S_k(G) - \left(-\partial_1^2\right)^k}{k!} + \sum_{k\geq k_0+1} \frac{1}{k!} \left(\sum_{i=2}^{n} \left|-\partial_i^2\right|\right)^k \\
&= \sum_{k=0}^{k_0} \frac{S_k(G) - \left(-\partial_1^2\right)^k}{k!} + \sum_{k\geq k_0+1} \frac{\left(2(1-\alpha)^2 \sum_{1\leq i<j\leq n} d_{ij}^2 + \alpha^2 \sum_{i=1}^{n} Tr_i^2 - \partial_1^2\right)^k}{k!} \\
&= \sum_{k=0}^{k_0} \frac{S_k(G) - \left(-\partial_1^2\right)^k}{k!} + e^{2(1-\alpha)^2 \sum_{1\leq i<j\leq n} d_{ij}^2 + \alpha^2 \sum_{i=1}^{n} Tr_i^2 - \partial_1^2} \\
&- \sum_{k=0}^{k_0} \frac{\left(2(1-\alpha)^2 \sum_{1\leq i<j\leq n} d_{ij}^2 + \alpha^2 \sum_{i=1}^{n} Tr_i^2 - \partial_1^2\right)^k}{k!},
\end{aligned}
$$

since

$$e^{2(1-\alpha)^2\sum_{1\le i<j\le n} d_{ij}^2+\alpha^2\sum_{i=1}^n Tr_i^2-\partial_1^2} = \sum_{k=0}^{k_0} \frac{\left(2(1-\alpha)^2\sum_{1\le i<j\le n} d_{ij}^2+\alpha^2\sum_{i=1}^n Tr_i^2-\partial_1^2\right)^k}{k!} + \sum_{k\ge k_0+1} \frac{\left(2(1-\alpha)^2\sum_{1\le i<j\le n} d_{ij}^2+\alpha^2\sum_{i=1}^n Tr_i^2-\partial_1^2\right)^k}{k!}.$$

Then the right hand side of Equation (4) follows. Again, from the derivation of the right hand side of Equation (4), it is evident that equality will be attained in the right hand side of Equation (4) if and only if G has no non-zero D_α-eigenvalues, i.e., $G = K_1$.

Next, we want to prove the left inequality. Since by Taylor's theorem $e^x \ge 1 + x$, equality holds if and only if $x = 0$, we have $e^{-\partial_i^2} \ge 1 - \partial_i^2$. Consequently,

$$P_\alpha(G) = \sum_{i=1}^n e^{-\partial_i^2} \ge \sum_{i=1}^n (1-\partial_i^2) = n - 2(1-\alpha)^2 \sum_{1\le i<j\le n} (d_{ij})^2 - \alpha^2 \sum_{i=1}^n Tr_i^2.$$

Hence, we get the left inequality. One can easily see that the left equality holds in Equation (4) if and only if $G = K_1$. □

Remark 1. *Assume that G is a connected graph of order n with diameter d. Since $d_{ij} \le d$ for $i \ne j$ and there are $\frac{n(n-1)}{2}$ pairs of vertices in G, also for each i, we have $Tr_i = Tr(v_i) \le \frac{n(n-1)}{2}$, then from the lower bound of Theorem 2, we see that*

$$\begin{aligned} P_\alpha(G) &\ge n - 2(1-\alpha)^2 \sum_{1\le i<j\le n} (d_{ij})^2 - \alpha^2 \sum_{i=1}^n Tr_i^2 \ge n - 2(1-\alpha)^2 \frac{n(n-1)}{2} d^2 - \alpha^2 \frac{n^3(n-1)^2}{4} \\ &= n - n(n-1)\left((1-\alpha)^2 d^2 + \alpha^2 \frac{n^2(n-1)}{4}\right). \end{aligned}$$

Next, we turn our attention to giving some lower bounds for the generalized distance Gaussian Estrada index $P_\alpha(G)$ through different graph invariants. The following result presents a lower bound in terms of the order n, the transmission degrees and the parameter $\alpha \in [0,1]$.

Theorem 3. *Suppose that G is a connected graph with order n and*

$$n \ge \max\left\{2\left(2(1-\alpha)^2 \sum_{1\le i<j\le n} d_{ij}^2 + \alpha^2 \sum_{i=1}^n Tr_i^2\right), \right. \left. 4(1-\alpha)^2 \sum_{1\le i<j\le n} d_{ij}^2 + 2\alpha^2 \sum_{i=1}^n Tr_i^2 - n(n-1)e^{-\frac{2(1-\alpha)^2\sum_{1\le i<j\le n} d_{ij}^2+\alpha^2\sum_{i=1}^n Tr_i^2}{n}} \right\}.$$

Then

$$P_\alpha(G) \ge \sqrt{n - 4(1-\alpha)^2 \sum_{1\le i<j\le n} (d_{ij})^2 - 2\alpha^2 \sum_{i=1}^n Tr_i^2 + n(n-1)e^{-\frac{4(1-\alpha)^2\sum_{1\le i<j\le n} d_{ij}^2+2\alpha^2\sum_{i=1}^n Tr_i^2}{n}}} \quad (5)$$

with equality if and only if $G = K_1$.

Proof. According to the definition of $P_\alpha(G)$, we have

$$P_\alpha^2(G) = \sum_{i=1}^{n} e^{-2\partial_i^2} + 2\sum_{i<j} e^{-\partial_i^2} e^{-\partial_j^2}. \tag{6}$$

By the arithmetic-geometric mean inequality, we obtain

$$\begin{aligned} 2\sum_{i<j} e^{-\partial_i^2} e^{-\partial_j^2} &\geq n(n-1)\left(\prod_{i>j} e^{-\partial_i^2} e^{-\partial_j^2}\right)^{\frac{2}{n(n-1)}} = n(n-1)\left[\left(\prod_{i=1}^{n} e^{-\partial_i^2}\right)^{n-1}\right]^{\frac{2}{n(n-1)}} \\ &= n(n-1)\left[\prod_{i=1}^{n} e^{-\partial_i^2}\right]^{\frac{2}{n}} = n(n-1)\left(e^{-\sum_{i=1}^{n}\partial_i^2}\right)^{\frac{2}{n}} \\ &= n(n-1)e^{-\frac{4(1-\alpha)^2\sum_{1\leq i<j\leq n} d_{ij}^2 + 2\alpha^2\sum_{i=1}^{n} Tr_i^2}{n}}. \end{aligned} \tag{7}$$

By means of a power-series expansion and noting that $S_0 = n$ and $S_1 = -2(1-\alpha)^2\sum_{1\leq i<j\leq n} d_{ij}^2 - \alpha^2\sum_{i=1}^{n} Tr_i^2$, we obtain

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

since $e^{-2\partial_i^2} \geq 1 - 2\partial_i^2$ holds for all i, and hence $\sum_{i=1}^{n} e^{-2\partial_i^2} \geq \sum_{i=1}^{n}(1-2\partial_i^2)$. If

$$n - 2\left(2(1-\alpha)^2\sum_{1\leq i<j\leq n} d_{ij}^2 + \alpha^2\sum_{i=1}^{n} Tr_i^2\right) \geq 0,$$

then we get $\sum_{i=1}^{n}\sum_{k\geq 2}\frac{\left(-2\partial_i^2\right)^k}{k!} \geq 0$. By substituting Equations (7) and (8) in Equation (6), we see that

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

This gives us the first part of the proof.

From the derivation of Equation (5), it is clear that equality holds if and only if the graph G has no non-zero D_α-eigenvalues. Since G is a connected graph, this only happens in the case of $G = K_1$. The proof is complete. □

As an immediate consequence of Theorem 3, we have the following corollary.

Corollary 2. *Let G be a connected graph of order n and with diameter d. Then*

$$P_\alpha(G) \geq \sqrt{n - n(n-1)\left(K - e^{-(n-1)K}\right)},$$

where $K = 2(1-\alpha)^2 d^2 + \frac{\alpha^2 n^2 (n-1)}{2}$. *Equality holds if and only if* $G = K_1$.

Proof. Since $\sum_{1\le i<j\le n}(d_{ij})^2 \le \frac{n(n-1)}{2}d^2$ and $\sum_{i=1}^{n} Tr_i^2 \le \frac{n^3(n-1)^2}{4}$, the result follows from Theorem 3. □

One of our main results in this paper is the following theorem, which gives a lower bound for $P_\alpha(G)$ involving the order n, transmission degrees, second transmission degrees and the parameter $\alpha \in [0,1]$. Moreover, it gives an upper bound via order n and the parameter $\alpha \in [0,1]$. It shows that, among all connected graphs of order n, the generalized distance Gaussian Estrada index takes its maximum for the complete graph.

Theorem 4. *Assume that G is a connected graph of order n. Then*

$$e^{-\frac{\sum_{i=1}^{n}(\alpha Tr_i^2+(1-\alpha)T_i)^2}{\sum_{i=1}^{n} Tr_i^2}} + (n-1)e^{\frac{\frac{\sum_{i=1}^{n}(\alpha Tr_i^2+(1-\alpha)T_i)^2}{\sum_{i=1}^{n} Tr_i^2} - \left(2(1-\alpha)^2\sum_{1\le i<j\le n} d_{ij}^2 + \alpha^2 \sum_{i=1}^{n} Tr_i^2\right)}{n-1}} \le P_\alpha(G)$$
$$\le e^{-(n-1)^2} + \frac{n-1}{e^{(\alpha n-1)^2}}. \tag{9}$$

The right equality holds if and only if $G = K_n$. Moreover, the left equality holds if and only if either G is a complete graph or for $\frac{1}{2} \le \alpha \le 1$, G is k-transmission regular graph with exactly three distinct D_α-eigenvalues

$$\left(2k, \sqrt{\frac{M+k^2(n\alpha^2-4)}{n-1}}, -\sqrt{\frac{M+k^2(n\alpha^2-4)}{n-1}}\right),$$

where $M = 2(1-\alpha)^2\sum_{1\le i<j\le n}(d_{ij})^2$.

Proof. We first consider the right-hand side inequality. Let $\partial_1 \ge \partial_2 \ge \ldots \ge \partial_n$ be the generalized distance eigenvalues of G. Note that by Corollary 1, we have $\partial_1 \ge Tr_{min} = n-1$. On the other hand, by Proposition 5 in [7] we get $\partial_n = \partial_n(G) \ge \partial_n(K_n) = \alpha n - 1$. Therefore

$$P_\alpha(G) = \sum_{i=1}^{n} e^{-\partial_i^2} \le \frac{1}{e^{(n-1)^2}} + \frac{(n-1)}{e^{\partial_n^2}} \le \frac{1}{e^{(n-1)^2}} + \frac{(n-1)}{e^{(\alpha n-1)^2}},$$

with equality if and only if G has exactly two distinct generalized distance eigenvalues $\partial_1 = n-1$ and $\partial_2 = \partial_3 = \cdots = \partial_n = \alpha n - 1$. Then by Lemma 3, we obtain $G = K_n$, and the proof is complete.

Next, we consider the left-hand side. According to the definition of $P_\alpha(G)$ and in view of the arithmetic-geometric mean inequality, we have

$$\begin{aligned} P_\alpha(G) &= e^{-\partial_1^2} + e^{-\partial_2^2} + \cdots + e^{-\partial_n^2} \\ &\ge e^{-\partial_1^2} + (n-1)\left(\prod_{i=2}^{n} e^{-\partial_i^2}\right)^{\frac{1}{n-1}} \qquad (10) \\ &= e^{-\partial_1^2} + (n-1)e^{\frac{-\sum_{i=2}^{n}\partial_i^2}{n-1}} \\ &= e^{-\partial_1^2} + (n-1)e^{\frac{\partial_i^2 - 2(1-\alpha)^2\sum_{1\le i<j\le n} d_{ij}^2 - \alpha^2\sum_{i=1}^{n} Tr_i^2}{n-1}}. \qquad (11) \end{aligned}$$

Consider the following function

$$f(x) = e^{-x} + (n-1)e^{\frac{x - 2(1-\alpha)^2\sum_{1\le i<j\le n} d_{ij}^2 - \alpha^2\sum_{i=1}^{n} Tr_i^2}{n-1}} \tag{12}$$

for $x \geq \frac{2(1-\alpha)^2 \sum_{1\leq i<j\leq n} d_{ij}^2 + \alpha^2 \sum_{i=1}^n Tr_i^2}{n}$. It is easy to see that $f(x)$ is an increasing function for $x \geq \frac{2(1-\alpha)^2 \sum_{1\leq i<j\leq n} d_{ij}^2 + \alpha^2 \sum_{i=1}^n Tr_i^2}{n}$. Since $2\sum_{1\leq i<j\leq n}(d_{ij})^2 < \frac{\left(\sum_{i=1}^n Tr_i\right)^2}{n}$, (see [32]) and $\sum_{i=1}^n T_i = \sum_{i=1}^n Tr_i^2$, also by the Cauchy-Schwartz inequality we have $\left(\sum_{i=1}^n T_i\right)^2 \leq n\sum_{i=1}^n T_i^2$ and $\left(\sum_{i=1}^n Tr_i\right)^2 \leq n\sum_{i=1}^n Tr_i^2$, and furthermore

$$\begin{aligned}
&\frac{2(1-\alpha)^2 \sum_{1\leq i<j\leq n}(d_{ij})^2 + \alpha^2 \sum_{i=1}^n Tr_i^2}{n} < \frac{\frac{(1-\alpha)^2\left(\sum_{i=1}^n Tr_i\right)^2}{n} + \alpha^2 \sum_{i=1}^n Tr_i^2}{n} \\
&\leq \frac{(1-\alpha)^2 \sum_{i=1}^n Tr_i^2 + \alpha^2 \sum_{i=1}^n Tr_i^2}{n} \leq \frac{\sum_{i=1}^n Tr_i^2}{n} \leq \frac{\left(\sum_{i=1}^n Tr_i^2\right)^2}{n\sum_{i=1}^n Tr_i^2} \\
&\leq \frac{\left(\sum_{i=1}^n(\alpha Tr_i^2 + (1-\alpha)T_i)\right)^2}{n\sum_{i=1}^n Tr_i^2} \leq \frac{\sum_{i=1}^n(\alpha Tr_i^2 + (1-\alpha)T_i)^2}{\sum_{i=1}^n Tr_i^2},
\end{aligned}$$

since

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

Therefore

$$\partial_1^2 \geq \frac{\sum_{i=1}^n(\alpha Tr_i^2 + (1-\alpha)T_i)^2}{\sum_{i=1}^n Tr_i^2} > \frac{2(1-\alpha)^2 \sum_{1\leq i<j\leq n}(d_{ij})^2 + \alpha^2 \sum_{i=1}^n Tr_i^2}{n}.$$

It follows from Equation (11) that

$$\begin{aligned}
P_\alpha(G) &\geq f\left(\frac{\sum_{i=1}^n(\alpha Tr_i^2 + (1-\alpha)T_i)^2}{\sum_{i=1}^n Tr_i^2}\right) \\
&= e^{-\frac{\sum_{i=1}^n(\alpha Tr_i^2+(1-\alpha)T_i)^2}{\sum_{i=1}^n Tr_i^2}} + (n-1)e^{\frac{\frac{\sum_{i=1}^n(\alpha Tr_i^2+(1-\alpha)T_i)^2}{\sum_{i=1}^n Tr_i^2} - \left(2(1-\alpha)^2 \sum_{1\leq i<j\leq n} d_{ij}^2 + \alpha^2 \sum_{i=1}^n Tr_i^2\right)}{n-1}}.
\end{aligned} \tag{13}$$

This completes the first part of the proof. Now, we suppose that the left equality holds in Equation (9). Then all inequalities in the above argument must be equalities. From Equation (13), we have $\partial_1 = \sqrt{\frac{\sum_{i=1}^n(\alpha Tr_i^2+(1-\alpha)T_i)^2}{\sum_{i=1}^n Tr_i^2}}$, which, by Lemma 2, implies that for $\frac{1}{2} \leq \alpha \leq 1$, G is a transmission regular graph. From Equation (10) and the arithmetic-geometric mean inequality, we get $\partial_2^2 = \partial_3^2 = \cdots = \partial_n^2$, then $|\partial_2| = \cdots = |\partial_n|$ and hence

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

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

$$|\partial_i| = \sqrt{\frac{P - \partial_1^2}{n-1}}, \quad i = 2, \ldots, n.$$

Hence, $|\partial_i|$ can have at most two distinct values and we arrive at the following classification:
(i) G has exactly one distinct D_α-eigenvalue. Then $G = K_1$.
(ii) G has exactly two distinct D_α-eigenvalues. Then, by Lemma 3, $G = K_n$.
(iii) G has exactly three distinct D_α-eigenvalues. Then $\partial_1 = \sqrt{\frac{\sum_{i=1}^n (\alpha Tr_i^2 + (1-\alpha)T_i)^2}{\sum_{i=1}^n Tr_i^2}}$ and $|\partial_i| = \sqrt{\frac{P - \frac{\sum_{i=1}^n (\alpha Tr_i^2 + (1-\alpha)T_i)^2}{\sum_{i=1}^n Tr_i^2}}{n-1}}$, $i = 2, \ldots, n$. Moreover, for $\frac{1}{2} \le \alpha \le 1$, G is k-transmission regular graph. Then it is clear that G is a graph with exactly three distinct D_α-eigenvalues

$$\left(2k, \sqrt{\frac{M + k^2(n\alpha^2 - 4)}{n-1}}, -\sqrt{\frac{M + k^2(n\alpha^2 - 4)}{n-1}}\right),$$

where $M = 2(1-\alpha)^2 \sum_{1 \le i < j \le n} (d_{ij})^2$. We have arrived at the desired result. □

This next result is for $P_\alpha(G)$. The parameters such as order n, Wiener index $W(G)$, transmission degrees and the parameter α are used.

Theorem 5. *Let G be a connected graph of order n and $0 \le \alpha \le \frac{2}{n+1}$. Then*

$$P_\alpha(G) \ge e^{-\frac{4W^2(G)}{n^2}} + (n-1)e^{\frac{\frac{4W^2(G)}{n^2} - \left(2(1-\alpha)^2 \sum_{1 \le i < j \le n} d_{ij}^2 + \alpha^2 \sum_{i=1}^n Tr_i^2\right)}{n-1}}. \tag{14}$$

Equality holds if and only if either G is a complete graph or a k-transmission regular graph with exactly three distinct D_α-eigenvalues

$$\left(2k, \sqrt{\frac{M + k^2(n\alpha^2 - 4)}{n-1}}, -\sqrt{\frac{M + k^2(n\alpha^2 - 4)}{n-1}}\right),$$

where $M = 2(1-\alpha)^2 \sum_{1 \le i < j \le n} (d_{ij})^2$.

Proof. By similar argument as in the proof of Theorem 4, we have

$$\begin{aligned} P_\alpha(G) &= e^{-\partial_1^2} + e^{-\partial_2^2} + \cdots + e^{-\partial_n^2} \\ &\ge e^{-\partial_1^2} + (n-1)\prod_{i=2}^n e^{-\frac{\sum_{i=2}^n \partial_i^2}{n-1}} \\ &= e^{-\partial_1^2} + (n-1)e^{\frac{\partial_i^2 - 2(1-\alpha)^2 \sum_{1 \le i < j \le n} d_{ij}^2 - \alpha^2 \sum_{i=1}^n Tr_i^2}{n-1}}. \end{aligned} \tag{15}$$

Consider the following function

$$f(x) = e^{-x} + (n-1)e^{\frac{x - 2(1-\alpha)^2 \sum_{1 \le i < j \le n} d_{ij}^2 - \alpha^2 \sum_{i=1}^n Tr_i^2}{n-1}}$$

for $x \geq \frac{2(1-\alpha)^2 \sum_{1\leq i<j\leq n} d_{ij}^2+\alpha^2 \sum_{i=1}^n Tr_i^2}{n}$. It is easy to see that $f(x)$ is an increasing function for $x \geq \frac{2(1-\alpha)^2 \sum_{1\leq i<j\leq n} d_{ij}^2+\alpha^2 \sum_{i=1}^n Tr_i^2}{n}$. Since $2\sum_{1\leq i<j\leq n}(d_{ij})^2 < \frac{\left(\sum_{i=1}^n Tr_i\right)^2}{n}$, (see [32]) also by the Cauchy-Schwartz inequality, we have

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

Hence,

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

Note that

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

since $(1-\alpha)^2+n\alpha^2 \leq 1$ for $0 \leq \alpha \leq \frac{2}{n+1}$. Therefore,

$$\partial_1^2 \geq \frac{4W^2(G)}{n^2} > \frac{2(1-\alpha)^2\sum_{1\leq i<j\leq n}(d_{ij})^2+\alpha^2\sum_{i=1}^n Tr_i^2}{n}. \tag{16}$$

It follows from Equation (15) that

$$P_\alpha(G) \;\; \geq \;\; f\left(\frac{4W^2(G)}{n^2}\right) = e^{-\frac{4W^2(G)}{n^2}}+(n-1)e^{\frac{\frac{4W^2(G)}{n^2}-\left(\frac{2(1-\alpha)^2\sum_{1\leq i<j\leq n}d_{ij}^2+\alpha^2\sum_{i=1}^n Tr_i^2}{n}\right)}{n-1}}.$$

The first part of the proof is complete. The remaining of the proof is similar to that of Theorem 4, and hence is omitted. □

Remark 2. *If we use* $P_\alpha(G) \geq f\left(\frac{2(1-\alpha)^2\sum_{1\leq i<j\leq n}(d_{ij})^2+\alpha^2\sum_{i=1}^n Tr_i^2}{n}\right)$ *instead in Equation (13), we are led to the following simpler estimation*

$$P_\alpha(G) \geq ne^{-\frac{2(1-\alpha)^2\sum_{1\leq i<j\leq n}(d_{ij})^2+\alpha^2\sum_{i=1}^n Tr_i^2}{n}},$$

with equality if and only if $G = K_1$.

Let $N(G) = \left(\prod_{i=1}^n Tr_i\right)^{\frac{1}{n}}$ be the geometric mean of the transmission degrees sequence. It can be seen that $\frac{2W(G)}{n} \geq N(G)$ holds, and equality is attained if and only if $Tr_1 = \cdots = Tr_n$ (i.e., the graph G is transmission regular).

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

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

We next establish a further lower bound for $P_\alpha(G)$ in terms of the order n, the geometric mean of the transmission degrees sequence $N(G)$, the Wiener index $W(G)$ and the parameter $\alpha \in [0,1]$.

Theorem 6. *Let G be a connected graph of order $n \geq 2$. Then*

$$P_\alpha(G)\geq e^{-\frac{4W^2(G)-N^2(G)n}{n(n-1)}}+(n-1)e^{\frac{\frac{4W^2(G)-N^2(G)n}{n(n-1)}-\left(2(1-\alpha)^2\sum_{1\leq i<j\leq n}d_{ij}^2+\alpha^2\sum_{i=1}^{n}Tr_i^2\right)}{n-1}}. \tag{17}$$

The equality holds if either G is a complete graph or a graph with exactly three distinct D_α-eigenvalues.

Proof. By similar argument as in the proof of Theorem 4 , we have

$$\begin{aligned}
P_\alpha(G) &= e^{-\partial_1^2}+e^{-\partial_2^2}+\cdots+e^{-\partial_n^2} \\
&\geq e^{-\partial_1^2}+(n-1)\prod_{i=2}^{n}e^{-\frac{\sum_{i=2}^{n}\partial_i^2}{n-1}} && (18)\\
&= e^{-\partial_1^2}+(n-1)e^{\frac{\partial_i^2-2(1-\alpha)^2\sum_{1\leq i<j\leq n}d_{ij}^2-\alpha^2\sum_{i=1}^{n}Tr_i^2}{n-1}}. && (19)
\end{aligned}$$

By Lemma 4, we see that $\partial_1 \geq \sqrt{\frac{\sum_{i=1}^{n}Tr_i^2}{n}}$. Setting $\sqrt{a_i} = Tr_i$ in Lemma 6, we have

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

Combining this with Lemma 4 yields

$$\partial_1\geq\sqrt{\frac{4W^2(G)-N^2(G)n}{n(n-1)}}. \tag{20}$$

It is easy to see that $\sqrt{\frac{4W^2(G)-N^2(G)n}{n(n-1)}} \geq \frac{2W(G)}{n}$, and so, by Equation (16), we have

$$\partial_1^2\geq\frac{4W^2(G)-N^2(G)n}{n(n-1)}\geq\frac{4W^2(G)}{n^2}>\frac{2(1-\alpha)^2\sum_{1\leq i<j\leq n}(d_{ij})^2+\alpha^2\sum_{i=1}^{n}Tr_i^2}{n}. \tag{21}$$

The remainder of the proof is similar to that of Theorem 4, and hence is omitted. □

Remark 3. *If we rely on the inequality $\frac{2W(G)}{n} \geq N(G)$, then we obtain*

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

Since the function $f(x)$ defined in Equation (12) is increasing, we see that our lower bound in Equation (17) is better than the given lower bound in Equation (14).

Let G be a k-transmission regular graph. Then it is clear that $W(G) = \frac{nk}{2}$ and $N(G) = k$. We have the following observation based upon Theorem 6.

Corollary 3. *Let G be a k-transmission regular graph. Then*

$$P_\alpha(G) \geq e^{-k^2} + (n-1)e^{\frac{k^2(1-n\alpha^2)-2(1-\alpha)^2\sum_{1\leq i<j\leq n}(d_{ij})^2}{n-1}},$$

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

4. Examples for Some Fundamental Special Graphs

In this section, we explicitly derive the exact values of $P_\alpha(G)$ for some fundamental special graphs including complete graphs, complete bipartite graphs, transmission regular graphs, regular graphs, cycles and various graphs generated by graph operations.

As mentioned in the 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 Section 3, we obtain the corresponding bounds for the distance Gaussian Estrada index $P^D(G)$ and the distance signless Laplacian Gaussian Estrada index $P^Q(G)$, respectively.

Since the generalized distance spectrum of K_n is $spec(K_n) = \{n-1, \alpha n - 1^{[n-1]}\}$, we have the following.

Lemma 7. *Let K_n be the complete graph of order n. Then*

$$P_\alpha(K_n) = e^{-(n-1)^2} + \frac{n-1}{e^{(\alpha n-1)^2}}.$$

Following [34], the generalized distance spectrum of the complete bipartite graph $K_{a,b}$ is

$$\begin{aligned} spec(K_{a,b}) \quad = \quad & \Big\{\alpha(2a+b) - 2^{[a-1]}, \alpha(2b+a) - 2^{[b-1]}, \frac{(\alpha+2)(a+b) - 4 + \sqrt{\eta}}{2}, \\ & \frac{(\alpha+2)(a+b) - 4 - \sqrt{\eta}}{2}\Big\}, \end{aligned}$$

where $\eta = (\alpha-2)^2(a^2+b^2) + 2ab(\alpha^2-2)$. We have the following expression for the $P_\alpha(G)$ of the complete bipartite graph.

Lemma 8. *Let $K_{a,b}$ be the complete bipartite graph of order $a+b$. Then*

$$P_\alpha(K_{a,b}) = (a-1)e^{-(\alpha(2a+b)-2)^2} + (b-1)e^{-(\alpha(2b+a)-2)^2} + e^{-\left(\frac{(\alpha+2)(a+b)-4+\sqrt{\eta}}{2}\right)^2} + e^{-\left(\frac{(\alpha+2)(a+b)-4-\sqrt{\eta}}{2}\right)^2},$$

where $\eta = (\alpha-2)^2(a^2+b^2) + 2ab(\alpha^2-2)$.

If we set $\alpha = 0$, the distance Gaussian Estrada index of $K_{a,b}$ is as follows.

Corollary 4.

$$P^D(K_{a,b}) = P_0(K_{a,b}) = (a+b-2)e^{-4} + e^{-\left(a+b-2+\sqrt{a^2+b^2-ab}\right)^2} + e^{-\left(a+b-2-\sqrt{a^2+b^2-ab}\right)^2}.$$

Moreover, if we set $\alpha = \frac{1}{2}$, the distance signless Laplacian Gaussian Estrada index of $K_{a,b}$ is as follows.

Corollary 5.

$$P^Q(K_{a,b}) = (a-1)e^{-(2a+b-4)^2} + (b-1)e^{-(2b+a-4)^2} + e^{-\left(\frac{5(a+b)-8+\sqrt{\eta}}{2}\right)^2} + e^{-\left(\frac{5(a+b)-8-\sqrt{\eta}}{2}\right)^2},$$

where $\eta = 9(a^2+b^2) - 14ab$.

The next result gives an expression for $P_\alpha(G)$ of a transmission regular graph G through the distance eigenvalues of G.

Theorem 7. *Let G be a k-transmission regular graph of order n having distance eigenvalues $\mu_1, \mu_2, \ldots, \mu_n$. Then*

$$P_\alpha(G) = e^{-\alpha^2 k^2} \sum_{i=1}^{n} e^{-(1-\alpha)\mu_i((1-\alpha)\mu_i + 2\alpha k)}.$$

Proof. Note that the generalized distance spectrum of the graph G reads as $\alpha k + (1-\alpha)\mu_1 \geq \alpha k + (1-\alpha)\mu_2 \geq \cdots \geq \alpha k + (1-\alpha)\mu_n$, where $\mu_1 \geq \cdots \geq \mu_n$ is the distance spectrum of G. Therefore,

$$P_\alpha(G) = \sum_{i=1}^{n} e^{-(\alpha k + (1-\alpha)\mu_i)^2} = e^{-\alpha^2 k^2} \sum_{i=1}^{n} e^{-(1-\alpha)\mu_i((1-\alpha)\mu_i + 2\alpha k)},$$

as desired. □

We next present an expression for $P_\alpha(G)$ of a regular graph G in terms of the adjacency eigenvalues of G.

Theorem 8. *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*

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

Proof. We know that the transmission of each vertex $v \in V(G)$ is $Tr(v) = d(v) + 2(n - d(v) - 1) = 2n - d(v) - 2$ and Wiener index $W(G)$ of G is $W(G) = n^2 - n - m$. Moreover,

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

where J is the all ones matrix. Therefore, we obtain

$$P_\alpha(G) = \sum_{i=1}^{n} e^{-\partial_i^2} = e^{-(2n-r-2)^2} + \sum_{i=2}^{n} e^{-(\alpha(2n+\lambda_i-r)-\lambda_i-2)^2},$$

as desired. □

Example 1. *Let C_n be a cycle of order n. Since C_n is a k-transmission regular graph with $k = \frac{n^2}{4}$ if n is even and $k = \frac{n^2-1}{4}$ if n is odd, then the generalized distance Gaussian Estrada index of C_n according to the parity of n, is as follows.*
If $n = 2p$ (i.e., n is even), then following [2] the distance spectrum of C_n is

$$spec(C_n) = \left\{0^{[p-1]}, \frac{n^2}{4}, -\csc^2\left(\frac{\pi(2j-1)}{n}\right)\right\} \quad for \quad j = 1, \ldots, p. \tag{22}$$

Hence, applying Theorem 7 we have

$$P_\alpha(C_n) = e^{-\frac{\alpha^2 n^4}{16}}\left(p - 1 + e^{\frac{(\alpha^2-1)n^4}{16}} + \sum_{j=1}^{p} e^{(1-\alpha)\csc^2\left(\frac{\pi(2j-1)}{n}\right)\left((\alpha-1)\csc^2\left(\frac{\pi(2j-1)}{n}\right)+\frac{\alpha n^2}{2}\right)}\right).$$

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

$$spec(C_n) = \left\{\frac{n^2-1}{4}, -\frac{1}{4}\sec^2\left(\frac{\pi j}{n}\right), -\frac{1}{4}\csc^2\left(\frac{\pi(2j-1)}{2n}\right)\right\} \quad for \quad j = 1, \ldots, p. \tag{23}$$

Hence, applying Theorem 7 we have

$$P_\alpha(C_n) = e^{-\frac{\alpha^2(n^2-1)^2}{16}}\left(e^{\frac{(\alpha^2-1)(n^2-1)^2}{16}} + \sum_{j=1}^{p} e^{\frac{(1-\alpha)\gamma_1}{4}\sec^2\left(\frac{\pi j}{n}\right)} + \sum_{j=1}^{p} e^{\frac{(1-\alpha)\gamma_2}{4}\csc^2\left(\frac{\pi(2j-1)}{2n}\right)}\right),$$

where $\gamma_1 = \frac{(\alpha-1)}{4}\sec^2\left(\frac{\pi j}{n}\right) + \frac{\alpha(n^2-1)}{2}$ and $\gamma_2 = \frac{(\alpha-1)}{4}\csc^2\left(\frac{\pi(2j-1)}{2n}\right) + \frac{\alpha(n^2-1)}{2}$.

Therefore, if we set $\alpha = 0$, the distance Gaussian Estrada index of C_n for $n = 2p$ is

$$P^D(C_n) = P_0(C_n) = p - 1 + e^{-\frac{n^4}{16}} + \sum_{j=1}^{p} e^{-\csc^4\left(\frac{\pi(2j-1)}{n}\right)},$$

and for $n = 2p + 1$ is

$$P^D(C_n) = P_0(C_n) = e^{-\frac{(n^2-1)^2}{16}} + \sum_{j=1}^{p} e^{-\frac{1}{16}\sec^4\left(\frac{\pi j}{n}\right)} + \sum_{j=1}^{p} e^{-\frac{1}{16}\csc^4\left(\frac{\pi(2j-1)}{n}\right)}.$$

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

Example 2. *Let G be an r-regular graph with an adjacency matrix A and adjacency spectrum $spec(G) = \{r, \lambda_2, \ldots, \lambda_n\}$. For any vertex $v \in G\nabla G$, 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 by [35] the graph $G\nabla G$ has distance spectrum $spec(G\nabla G) = \left\{3n-r-2, n-r-2, -2(\lambda_i+2)^{[2]}\right\}$, for $i = 2, \ldots, n$. By Theorem 7, we have

$$P_\alpha(G\nabla G) = e^{-\alpha^2(3n-r-2)^2}\left(e^{(\alpha-1)(n-r-2)\sigma_1} + e^{(\alpha-1)(3n-r-2)\sigma_2} + 2\sum_{i=2}^{n} e^{2(1-\alpha)(\lambda_i+2)\sigma_3}\right),$$

where $\sigma_1 = \alpha(5n-r-2) + n - r - 2$, $\sigma_2 = (\alpha+1)(3n-r-2)$ and $\sigma_3 = 2\alpha(\lambda_i + 3n - r) - 2\lambda_i - 4$. Therefore, if we set $\alpha = 0$, the distance Gaussian Estrada index of $G\nabla G$ is

$$P^D(G\nabla G) = P_0(G\nabla G) = e^{-(n-r-2)^2} + e^{-(3n-r-2)^2} + 2\sum_{i=2}^{n} e^{-4(\lambda_i+2)^2}.$$

If we set $\alpha = \frac{1}{2}$, the distance signless Laplacian Gaussian Estrada index of $G\nabla G$ is

$$P^Q(G\nabla G) = e^{-(3n-r-2)^2}\left(e^{-(n-r-2)\sigma_1} + e^{-(3n-r-2)\sigma_2} + 2\sum_{i=2}^{n} e^{2(\lambda_i+2)\sigma_3}\right),$$

where $\sigma_1 = 7n - 3r - 6$, $\sigma_2 = 3(3n-r-2)$ and $\sigma_3 = 2(3n - \lambda_i - r - 4)$.

The cartesian product of two graphs G_1 and G_2 is denoted by $G_1 \times G_2$. The cartesian product can be viewed as a graph with vertex set $V(G_1) \times V(G_2)$ and edge set containing all edges $\{(u_1, u_2), (v_1, v_2)\}$ such that $u_1 = v_1$ and $u_2v_2 \in E(G_2)$ or $u_2 = v_2$ and $u_1v_1 \in E(G_1)$.

Example 3. *Let G be an r-regular graph of diameter at most 2 with an adjacency matrix A and adjacency spectrum $spec(G) = \{r, \lambda_2, \ldots, \lambda_n\}$, and let $H = G \times K_2$. Suppose $V(G) = \{v_1, v_2, \ldots, v_n\}$ and $V(K_2) = \{w_1, w_2\}$. From the fact $d_H((v_i, w_j), (v_s, w_t)) = d_G(v_i, v_s) + d_{K_2}(w_j, w_t) = d_G(v_i, v_s) + 1$, we see that all vertices of H have the same transmission and $Tr_H(v_i, w_j) = 5n - 2r - 4$. So $Tr(H) = (5n-2r-4)I$. Note that by [35], the graph $H = G \times K_2$ has distance spectrum $spec(H) = \left\{5n - 2(r+2), -2(\lambda_i+2), -n, 0^{[n-1]}\right\}$, for $i = 2, \ldots, n$. Then by Theorem 7, we have*

$$P_\alpha(H) = e^{-\alpha^2(5n-2r-4)^2}\left(n - 1 + e^{n(1-\alpha)\xi_1} + e^{(\alpha^2-1)(5n-2r-4)^2} + \sum_{i=2}^{n} e^{4(1-\alpha)(\lambda_i+2)\xi_2}\right),$$

where $\xi_1 = \alpha(11n - 4r - 8) - n$ and $\xi_2 = \alpha(\lambda_i + 5n - 2r - 2) - \lambda_i - 2$. Therefore, if we set $\alpha = 0$, the distance Gaussian Estrada index of $H = G \times K_2$ is

$$P^D(H) = P_0(H) = n - 1 + e^{-n^2} + e^{-(5n-2r-4)^2} + \sum_{i=2}^{n} e^{-4(\lambda_i+2)^2}.$$

If we set $\alpha = \frac{1}{2}$, the distance signless Laplacian Gaussian Estrada index of $H = G \times K_2$ is

$$P^Q(H) = e^{-(5n-2r-4)^2}\left(n - 1 + e^{n\xi_1} + e^{-3(5n-2r-4)^2} + \sum_{i=2}^{n} e^{4(\lambda_i+2)\xi_2}\right),$$

where $\xi_1 = 9n - 4r - 8$ and $\xi_2 = 5n - \lambda_i - 2r - 6$.

Now, we give an expression for the generalized distance Gaussian Estrada index of the lexicographic product $G[H]$ built upon two graphs G and H.

Definition 1. *[1]* 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 $V(H)$, in which $u = (u_1, v_1)$ 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.

Example 4. *Let G be a k-transmission regular graph of order p. Let H be an r-regular graph of order n with adjacency eigenvalues $\{r, \lambda_2, \ldots, \lambda_n\}$. Let $\{\mu_1, \ldots, \mu_p\}$ be the eigenvalues of the distance matrix $D(G)$ of G. 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 by [36], the graph $G[H]$ has distance spectrum $spec(G[H]) = \left\{n\mu_i + 2n - r - 2, -2(\lambda_j + 2)^{[n]}\right\}$, for $i = 1, \ldots, p$ and $j = 2, \ldots, n$. In view of Theorem 7, we have*

$$P_\alpha(G[H]) = e^{-\alpha^2(kn+2n-r-2)^2} \left(\sum_{i=1}^{p} e^{(\alpha-1)(n\mu_i+2n-r-2)\zeta_1} + n \sum_{j=2}^{n} e^{4(1-\alpha)(\lambda_i+2)\zeta_2} \right),$$

where $\zeta_1 = \alpha(2kn - n\mu_i + 2n - r - 2) + n\mu_i + 2n - r - 2$ and $\zeta_2 = \alpha(kn + \lambda_i + 2n - r) - \lambda_i - 2$. Similarly, if we set $\alpha = 0$, the distance Gaussian Estrada index of $G[H]$ is

$$P^D(G[H]) = P_0(G[H]) = \sum_{i=1}^{p} e^{-(n\mu_i+2n-r-2)^2} + n \sum_{j=2}^{n} e^{-4(\lambda_i+2)^2}.$$

If we set $\alpha = \frac{1}{2}$, the distance signless Laplacian Gaussian Estrada index of $G[H]$ is

$$P^Q(G[H]) = e^{-(kn+2n-r-2)^2} \left(\sum_{i=1}^{p} e^{-(n\mu_i+2n-r-2)\zeta_1} + n \sum_{j=2}^{n} e^{4(\lambda_i+2)\zeta_2} \right),$$

where $\zeta_1 = 2kn + n\mu_i + 6n - 3r - 6$ and $\zeta_2 = kn - \lambda_i + 2n - r - 4$.

We conclude by computing the generalized distance Gaussian Estrada index of the closed fence graph.

Example 5. *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 Example 4, we will be able to compute the generalized distance Gaussian Estrada index of closed fence $G = C_n[K_2]$. It is well known that the adjacency spectrum of the graph K_2 is $spec(K_2) = \{1, -1\}$. Then, applying Example 4, the generalized distance Gaussian 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 by Equation (22) and applying Example 4 we have

$$P_\alpha(C_n[K_2]) = e^{-\alpha^2\left(\frac{n^2}{2}+1\right)^2}\Bigg((z-1)e^{(\alpha-1)m_1} + e^{(\alpha-1)\left(\frac{n^2}{2}+1\right)m_2} + \sum_{j=1}^{z} e^{(\alpha-1)\left(-2\csc^2\left(\frac{\pi(2j-1)}{n}\right)+1\right)m_3}$$
$$+ \; 2e^{4(1-\alpha)m_4}\Bigg),$$

where $m_1 = \alpha(n^2+1)+1$, $m_2 = (\alpha+1)\left(\frac{n^2}{2}+1\right)$, $m_3 = \alpha\left(n^2+2\csc^2\left(\frac{\pi(2j-1)}{n}\right)+1\right) - 2\csc^2\left(\frac{\pi(2j-1)}{n}\right)+1$ *and* $m_4 = \alpha\left(\frac{n^2}{2}+2\right)-1$.

If $n = 2z+1$ *(i.e., n is odd), then by Equation (23) and applying Example 4 we have*

$$P_\alpha(C_n[K_2]) = e^{-\alpha^2\left(\frac{n^2+1}{2}\right)^2}\Bigg(e^{(\alpha-1)\left(\frac{n^2+1}{2}\right)h_1} + \sum_{j=1}^{z} e^{(\alpha-1)\left(-\frac{1}{2}\sec^2\left(\frac{\pi j}{n}\right)+1\right)h_2} + \sum_{j=1}^{z} e^{(\alpha-1)\left(-\frac{1}{2}\csc^2\left(\frac{\pi(2j-1)}{2n}\right)+1\right)h_3}$$
$$+ \; 2e^{4(1-\alpha)m_4}\Bigg),$$

where $h_1 = \alpha\left(\frac{n^2+3}{2}\right) + \frac{n^2+1}{2}$, $h_2 = \alpha\left(n^2+1-\frac{1}{2}\sec^2\left(\frac{\pi j}{n}\right)\right) - \frac{1}{2}\sec^2\left(\frac{\pi j}{n}\right)+1$, $h_3 = \alpha\left(n^2+1-\frac{1}{2}\csc^2\left(\frac{\pi(2j-1)}{2n}\right)\right) - \frac{1}{2}\csc^2\left(\frac{\pi(2j-1)}{2n}\right)+1$ *and* $m_4 = \alpha\left(\frac{n^2}{2}+2\right)-1$.

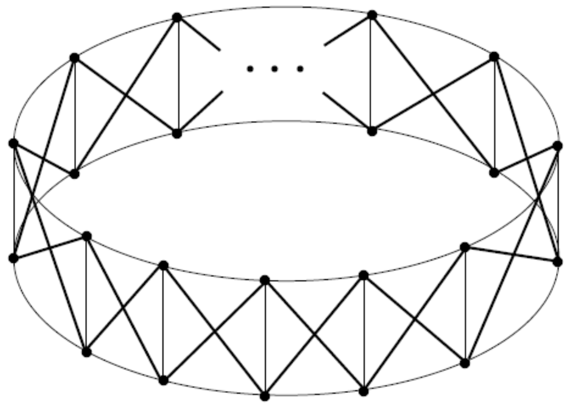

Figure 1. The closed fence graph.

5. 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. It has attracted increasing attention in recent years and has been extended to varied forms involving many of the important graph matrices such as the Laplacian matrix and distance matrix. The recently introduced Gaussian Estrada index $H(G)$ [26] has the merit of encoding the information hidden in the eigenvalues close to zero which are overlooked in other Estrada indices. It has also played an essential role in quantum mechanics [27].

In this paper we have proposed a new sort of Estrada index based upon the Gaussianization of the generalized distance matrix of a graph. Let $\partial_1, \partial_2, \ldots, \partial_n$ be the generalized distance eigenvalues of a graph G. We defined the generalized distance Gaussian Estrada index as $P_\alpha(G) = \sum_{i=1}^{n} e^{-\partial_i^2}$, which reduces to merging the spectral theories of Gaussian Estrada index with respect to distance matrix and Gaussian Estrada index with respect to distance signless Laplacian matrix, and any result regarding the spectral properties of generalized distance Gaussian Estrada index has its counterpart for each of these particular indices, and these counterparts follow immediately from a single proof. Since characterization of $P_\alpha(G)$ turns out to be highly desirable in quantum information theory, it is interesting to study the quantity $P_\alpha(G)$ 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 Gaussian Estrada index $P_\alpha(G)$ of a connected graph G through the different graph parameters including the order n, the Wiener index $W(G)$, the transmission degrees and the parameter $\alpha \in [0,1]$. We have also characterized the extremal graphs attaining these bounds. Some expressions for $P_\alpha(G)$ of some fundamental special graphs have been worked out.

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