

ON THE DEGREE DISTANCE MATRIX OF CONNECTED  
GRAPHS

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ABSTRACT. Let  $d_u$  denote the degree of vertex  $u$  and  $d_{uv}$  be the distance between vertices  $u$  and  $v$  in a connected graph  $G$ . We propose studying the degree distance matrix of a connected graph  $G$ , defined as  $M_{DD}(G) = ((d_u + d_v)d_{uv})_{u,v \in V(G)}$ . This study sheds new light on the spectra of degree and distance-based matrices. Some spectral properties of  $M_{DD}(G)$  are given along with some open problems that can help to understand the degree distance matrix in depth. Furthermore,  $M_{DD}$  spectra of some graphs are obtained. Moreover, an effort is made to get some sharp lower and upper bounds for the  $M_{DD}$  spectral radius.

## 1. INTRODUCTION

Throughout this paper we consider simply connected undirected graphs. Let  $G$  be a graph of order  $n$  with vertex set  $V(G)$  and edge set  $E(G)$ . For  $u, v \in V(G)$ , we define the *distance* between vertex  $u$  and  $v$  in  $G$ , denoted by  $d(u, v)$  or for simplicity  $d_{uv}$ , is the length of a shortest path from vertex  $u$  to vertex  $v$  in  $G$ . The maximum distance between any two vertices in  $G$  is called *diameter* of  $G$ , denoted by  $\mathbf{d}(G)$ . Two vertices  $u, v \in G$  are said to be *adjacent* if they share the same edge, i.e.,  $u \sim v$ . For  $u \in G$  the number of vertices adjacent to  $u$  is defined as *degree of vertex  $u$*  and denoted as  $d_u$ . A graph  $G$  is said to be a  *$k$ -regular graph* if each vertex of  $G$  has degree  $k$ . The *distance matrix* of  $G$  is  $n \times n$  matrix  $D(G) = (d_{uv})_{u,v \in V(G)}$ . For  $u \in V(G)$ , the *transmission* of  $u$  (also known as degree distance of  $u$ ) in  $G$ , denoted by  $Tr_u$ , is defined as the sum of distances from  $u$  to all other vertices of  $G$ , i.e.,  $Tr_u(G) = \sum_{v \in V(G)} d_{uv}$ . A connected graph  $G$  is said to be  *$r$ -transmission regular* if for each  $v \in V(G)$ ,  $Tr(v) = r$ . We define the degree transmission of vertex  $u \in V(G)$  as  $T_u^D(G) = \sum_{v \in V(G)} d_v d_{uv}$ . A graph  $G$  is said to be

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*vertex degree transmission regular* if for each vertex  $v \in V(G)$ ,  $d_v = k$  and  $Tr_v = r$ . It is clear that any vertex-transitive graph (a graph  $G$  in which for every two vertices  $u$  and  $v$ , there exists an automorphism  $f$  on  $G$  such that  $f(u) = v$ ) is a vertex degree and transmission regular graph. By definition, a vertex degree regular graph is obviously a transmission regular graph, but a transmission regular graph may not be a vertex degree regular graph. In [3], authors have discussed some transmission regular but not vertex degree regular graphs.

The study of the distance matrix is of great significance and interest. Consonni and Todeschini [2] briefly studied and proposed that the degree distance spectral radius is widely applicable as a molecular descriptor in QSPR modeling. The distance eigenvalues and especially the distance spectral radius have been extensively studied for the last many years, see the recent survey [1] along with references therein and [4, 5, 6, 7, 8]. In [12], Dobrynin and Kochetova introduced a degree and distance-based molecular index for graphs called the degree distance index. In chemical graph theory literature, degree distance index  $\mathbb{D}_{\mathbb{I}}$  was investigated by Tomescu [13] [14], Bucicovschi and Cioabă [15]. For any  $i, j \in V(G)$  the degree distance index of connected graph  $G$  is defined as,

$$\mathbb{D}_{\mathbb{I}}(G) = 2 \sum_{i < j} (d_i + d_j) d_{ij}$$

The indices are widely used in mathematical chemistry as the graphs usually represent the perfect atomic or molecular model structures. In [16], well-known chemist O. Ivanciuc studied the distance valency matrices and derived molecular graph descriptors, where he defined the degree distance valency matrix for his molecular graph descriptors. The distance valency matrices are very flexible in representing the chemical structure in numerical form with efficient use in different structural properties and molecular studies. Using molecular graphs, one can easily determine the structure of various chemical compounds from their spectral moment, spectra, polynomials, walks and paths. For more details on molecular indices and their applications, readers are suggested to see [9], [10] and [11].

In this paper, using the concept of degree distance index [12] and valency matrices [16] we investigate a degree distance matrix. Let  $G$  be a connected graph of order  $n$  then the degree distance matrix for any connected graph is defined as  $M_{DD}(G) = (m_{ij})$ , where

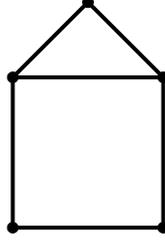
$$m_{ij} = \begin{cases} (d_i + d_j) d_{ij}, & \text{if } i \neq j, \\ 0, & \text{otherwise.} \end{cases}$$

As  $G$  is connected so it's obvious from the definition of degree distance matrix that  $m_{ij} \geq 2$  for  $i \neq j$  and  $m_{ii} = 0$ . Let  $\lambda_1 \geq \lambda_2 \geq \dots \geq \lambda_n$  be the nonincreasing eigenvalues of  $M_{DD}(G)$ , where  $\lambda_1$  is the maximum eigenvalue known as *degree distance spectral radius* and will be denoted by  $\rho(G)$ . Let

$\mathbb{D}_i$  be the sum of the  $i$ th row or column of  $M_{DD}(G)$ , then clearly

$$\mathbb{D}_{\mathbb{I}}(G) = \frac{1}{2} \sum_{i=1}^n \mathbb{D}_i.$$

**Example 1.1.** Let  $G_1$  be a graph on 5 vertices. We can write  $M_{DD}$  of  $G_1$  as:



$G_1$

$$M_{DD}(G_1) = \begin{bmatrix} 0 & 5 & 8 & 10 & 4 \\ 5 & 0 & 5 & 6 & 10 \\ 8 & 5 & 0 & 5 & 8 \\ 10 & 6 & 5 & 0 & 5 \\ 4 & 10 & 8 & 5 & 0 \end{bmatrix}$$

The degree distance spectrum of  $G_1$  can be calculated from the above matrix, i.e.,

$$\text{Spec}(M_{DD}(G_1)) = \left( \begin{array}{ccccc} \lambda_1 & \lambda_2 & \lambda_3 & \lambda_4 & \lambda_5 \\ 26.41 & 0.01 & -4.95 & -10.11 & -11.82 \end{array} \right)$$

The remaining sections of the paper are organized as follows. In section 2, some basic properties of  $M_{DD}(G)$  and the degree distance spectral radius are given. In section 3, we focus on degree distance spectra of some graphs and determine the degree distance spectra of graphs obtained by certain graph operations. In section 4, we focus on sharp upper and lower bounds for the degree distance spectral radius  $\rho(M_{DD}(G))$ . Section 5 of the paper is dedicated to a discussion, where upper and lower bounds for some connected graphs are compared.

## 2. BASIC PROPERTIES OF THE DEGREE DISTANCE MATRIX

Let  $G$  be a connected graph with  $V(G) = \{v_1, \dots, v_n\}$  and a column vector  $x = (x_1, \dots, x_n)^T \in \mathbb{R}^n$  can be considered as a function defined on  $V(G)$ , which maps vertex  $v_i$  to  $x_i$ , i.e.,  $x(v_i) = x_i$  for  $i = 1, \dots, n$ . Then

$$x^T M_{DD}(G)x = \sum_{i=1}^n \sum_{j=1}^n (d_i + d_j) d_{ij} x_i x_j,$$

or equivalently,

$$x^T M_{DD}(G)x = 2 \sum_{i < j} (d_i + d_j) d_{ij} x_i x_j,$$

Here we recall that a matrix is *irreducible* if it cannot be placed into block upper-triangular form by simultaneous row/column permutations. Since  $M_{DD}(G)$  is a nonnegative irreducible matrix, by the Perron–Frobenius theorem,  $\rho(G)$  is simple and there is a unique positive unit eigenvector corresponding to  $\rho(G)$ , which is called the *DD-Perron vector* of  $G$ . If  $x$  is the *DD-Perron vector* of  $G$ , then for each  $i \in V(G)$ ,

$$\rho(G)x_i = \sum_{j=1}^n ((d_i + d_j) d_{ij}) x_j,$$

or equivalently,

$$\rho(G)x_i = d_i \sum_{j=1}^n d_{ij} x_j + \sum_{j=1}^n d_j d_{ij} x_j$$

is called *degree distance eigenequation* (*DD-eigenequation*) of  $G$  at vertex  $i$ . For a unit column vector  $x \in \mathbb{R}^n$  with at least one nonnegative entry, by Rayleigh’s principle, we have  $\rho(G) \geq x^T M_{DD}(G)x$  with equality if and only if  $x$  is the *DD-Perron vector* of  $G$ .

Since  $M_{DD}(G)$  is a nonnegative irreducible matrix, so by the Perron–Frobenius theorem we have following properties:

**Lemma 2.1.** *Let  $G$  be a connected graph of order  $n$ . Let  $x$  be an eigenvector corresponding to  $\rho(G)$ . Then*

- $\rho(G)$  is the maximum eigenvalue and has multiplicity 1;
- the eigenvector  $x$  is positive and unique up to scaling;
- if  $G^*$  is a spanning subgraph of  $G$ , then

$$\rho(G^*) \leq \rho(G).$$

**Lemma 2.2.** *Let  $G$  be a graph of order  $n$  and let  $\lambda_1, \lambda_2, \dots, \lambda_n$  be its degree distance eigenvalues. Then,*

- (1)  $\sum_{i=1}^n \lambda_i = 0$ ;
- (2)  $\sum_{i=1}^n \lambda_i^2 = 2\mathcal{S}$ , where  $\mathcal{S} = \sum_{i < j} ((d_i + d_j) d_{ij})^2$ .

*Proof.* Let  $G$  be a connected graph with  $n$  vertices. Since,  $\sum_{i=1}^n \lambda_i = \text{trace}[M_{DD}]$  but in case of the degree distance matrix  $m_{ii} = 0$ , therefore,  $\sum_{i=1}^n \lambda_i = 0$ .

Now for the second equality, let  $i = 1, 2, \dots, n$  then the  $(i, i)$ th entry of the  $[M_{DD}]^2$  equals  $\sum_{i=1}^n ((d_i + d_j) d_{ij})^2$ . As  $M_{DD}$  is a symmetric matrix, therefore

$$\sum_{i=1}^n \lambda_i^2 = \text{trace}[M_{DD}(G)]^2 = \sum_{i=1}^n \sum_{j=1}^n ((d_i + d_j) d_{ij})^2$$

$$\implies \sum_{i=1}^n \lambda_i^2 = 2 \sum_{i < j} ((d_i + d_j)d_{ij})^2 = 2\mathcal{S}.$$

□

Two vertices  $u$  and  $v$  are equivalent in a connected graph  $G$  if there exists an automorphism  $\sigma : G \rightarrow G$ , such that  $\sigma(u) = v$ . In the next proposition we will use the vertex equivalence property to obtain an important property of the eigenvector corresponding to  $\rho(G)$ .

**Proposition 2.3.** *Let  $G$  be a connected graph of order  $n$  and  $u, v \in V(G)$ . Let  $x = (x_1, x_2, \dots, x_n)^T$  be an eigenvector corresponding to  $\rho(G)$ . If vertices  $u$  and  $v$  are equivalent in  $G$ , then  $x_u = x_v$ .*

*Proof.* Let  $G$  be a connected graph of order  $n$ . Since  $u, v \in V(G)$  and vertices  $u$  and  $v$  are equivalent in  $G$ , then there exists a permutation matrix  $P$  such that  $P^{-1}M_{DD}(G)P = M_{DD}(G)$ . Thus  $P^{-1}M_{DD}(G)Px = \rho(M_{DD}(G))x$ . It follows that  $Px$  is also an eigenvector of  $\rho(M_{DD}(G))$ , which is a contradiction to Proposition 2.1 that  $x$  is unique. So,  $Px = x$  and  $x_u = x_v$ . □

Recall that a connected graph  $G$  is said to be a  $k$ -regular graph if for each vertex  $v \in G$ ,  $d_v = k$ . If  $D$  is the distance matrix of  $G$ , then we clearly see that for a  $k$ -regular graph the degree distance matrix can be written as  $M_{DD}(G) = 2kD(G)$ . This leads us to the following lemma.

**Lemma 2.4.** *Let  $G$  be a connected  $k$ -regular graph on  $n$  vertices. Let  $D$  be the distance matrix of  $G$  with eigenvalues  $\mu_1 \geq \mu_2 \geq \dots \geq \mu_n$ . Then the degree distance spectrum of  $G$  is  $2k\mu_i$ , where  $i = 1, 2, \dots, n$ .*

### 3. DEGREE DISTANCE SPECTRA OF SOME GRAPHS

**Lemma 3.1** ([18]). *Let  $M$  be a Hermitian matrix of order  $r$ , and let  $N$  be the principal submatrix of  $M$  with order  $s$ . If  $\lambda_1 \geq \lambda_2 \geq \dots \geq \lambda_r$  are the eigenvalues of  $M$  and  $\mu_1 \geq \mu_2 \geq \dots \geq \mu_s$  are the eigenvalues of  $N$ , then  $\lambda_i(G) \geq \mu_i \geq \lambda_{r-s+i}$  for  $1 \leq i \leq s$ .*

Our next lemma will give us a better understanding of the minimum and maximum eigenvalues of the degree distance matrix corresponding to the diameter  $\mathbf{d}$  of a graph.

**Lemma 3.2.** *Let  $G$  be an  $n$ -vertex connected graph with diameter  $\mathbf{d}$ . Then  $\lambda_1(G) \geq 2\mathbf{d}(G)$  and  $\lambda_n(G) \leq -2\mathbf{d}(G)$ .*

*Proof.* Let  $G$  be an  $n$ -vertex connected graph. If  $n = 1$  then the case is obvious as  $\lambda_1(G) = 0$ . Let  $n \geq 2$  and consider a diametrical path  $P = u_1u_2 \dots u_{d+1}$  in  $G$ . Then we see that the distance  $d(u_1, u_{d+1}) = \mathbf{d}$ . From the definition of the degree distance matrix, we see that the entry  $u_1u_{d+1}$  (resp.  $u_{d+1}u_1$ ) =  $(d_{u_1} + d_{u_{d+1}})d_{u_1u_{d+1}} \geq 2\mathbf{d}$ . Lets assume

$d_{u_1} = d_{u_{d+1}} = 1$ . Hence,  $C = \begin{pmatrix} 0 & 2\mathbf{d} \\ 2\mathbf{d} & 0 \end{pmatrix}$  is the principal submatrix of  $M_{DD}(G)$  with corresponding eigenvalues  $\mu_1 = 2\mathbf{d}$  and  $\mu_2 = -2\mathbf{d}$ . From Lemma 3.1, we get  $\lambda_1(G) \geq \mu_1 = 2\mathbf{d}$  and  $\lambda_n(G) \leq \mu_2 = -2\mathbf{d}$ .  $\square$

**Theorem 3.3.** *Let  $G$  be a graph on  $n$  vertices. Then  $\lambda_n(G) = -2(n-1)$  if and only if  $G$  is a complete graph.*

*Proof.* For the sufficiency of the theorem, assume  $G \equiv K_n$ . Then  $\lambda_n(K_n) = -2(n-1)$  as desired.

Now, for the necessity condition, let  $G$  be a connected graph of order  $n$  and assume that  $\lambda_n(G) = -2(n-1)$ . If diameter  $\mathbf{d} > 1$ , then from Lemma 3.2  $\lambda_n(G) \leq -2\mathbf{d} < -2(n-1)$ , a contradiction. So we consider that the diameter of  $G$  is 1 and this implies that  $G \equiv K_n$ . By proving the sufficient and necessary condition, we have  $\lambda_n(K_n) = -2(n-1)$ , as required.  $\square$

**Lemma 3.4.** *A connected graph  $G$  has two distinct  $M_{DD}$  eigenvalues if and only if  $G$  is a complete graph.*

*Proof.* The proof is partially similar to Lemma 2 of [19]. Let  $G$  be a connected graph with degree distance matrix  $M_{DD}(G)$ . Assume that  $\lambda_1$  and  $\lambda_2$  are the only two distinct eigenvalues of  $G$ , where  $\lambda_1 > \lambda_2$ . Since  $G$  is connected and irreducible, by the Perron–Frobenius theorem,  $\lambda_1$  is the maximum eigenvalue and has multiplicity 1. Thus the remaining  $n-1$  eigenvalues of  $G$  are  $\lambda_2$ . Now we will show that the diameter of  $G$  is 1.

Suppose  $G$  contains an induced path  $P_l, l \geq 3$ . Let  $A$  be a principal submatrix of  $M_{DD}$ . Let  $\mu_i(A)$  be the  $i$ th eigenvalue of  $A$ , then by the interlacing theorem we have,

$$\lambda_2 \geq \mu_2(A) \geq \mu_3(A) \geq \cdots \geq \mu_l(A) \geq \mu_n(A) = \lambda_2$$

This clearly shows that  $P_l$  has at most two distinct  $M_{DD}$  eigenvalues for  $l \geq 3$ , a contradiction. Hence,  $G$  has diameter 1 and is a complete graph.

Conversely, assume that  $G$  is a complete graph ( $K_n$ ) of order  $n$ . Then  $M_{DD}(K_n)$  has diagonal entries 0 and nondiagonal entries  $2(n-1)$ . Let  $J$  be the all-one matrix and  $I$  be the identity matrix both of order  $n$  then  $M_{DD}(K_n) = 2(n-1)(J - I)_{n \times n}$ . So,  $G$  has exactly two distinct  $M_{DD}$  eigenvalues  $2(n-1)^2$  with multiplicity 1 and  $-2(n-1)$  with multiplicity  $n-1$ .  $\square$

**Lemma 3.5** ([20]). *Let*

$$B = \begin{bmatrix} B_0 & B_1 \\ B_1 & B_0 \end{bmatrix}$$

*be a  $2 \times 2$  block symmetric matrix. Then the eigenvalues of  $B$  are those of  $B_0 + B_1$  with those of  $B_0 - B_1$ .*

**Definition 3.6** ([21]). *Let  $G$  be a connected graph with vertex set  $V(G) = \{u_1, u_2, \dots, u_n\}$ . Let  $N(u_i)$  be the set of vertices adjacent to  $u_i$ . Take another copy of  $G$  with vertex set  $\{v_1, v_2, \dots, v_n\}$ , where each  $v_i$  corresponds*

to vertex  $v_i$  for  $i = 1, 2, \dots, n$ . Make  $v_i$  adjacent to all vertices in  $N(u_i)$  in  $G$  for each  $i$ . The resulting graph is called a double of graph  $G$  and denoted by  $D_2G$ .

**Theorem 3.7** ([23]). *Let  $G$  be connected graph on  $n$  vertices with distance spectrum  $\mu_1 \geq \mu_2 \geq \dots \mu_n$ . Then*

$$\text{spec}_D(D_2G) = \begin{pmatrix} 2(\mu_i + 1) & -2 \\ 1 & n \end{pmatrix}, i = 1, 2, \dots, n$$

Next, using the concept of Theorem 3.7 we present the proof for the degree distance spectra of a double of a graph.

**Theorem 3.8.** *Let  $G$  be a connected graph on  $n$  vertices and let degree distance spectrum of  $G$  be  $\text{spec}_{M_{DD}}(G) = \{\lambda_1, \lambda_2, \dots, \lambda_n\}$ . Let  $\text{diag}(d_{u_i})$  be  $n \times n$  diagonal matrix with diagonal entries as degrees of vertices  $u_i$ , where  $i = 1, 2, \dots, n$ . Then*

$$\text{spec}_{M_{DD}}(D_2G) = \begin{pmatrix} 4\lambda'_i & -8d_{u_i}(G) \\ 1 & 1 \end{pmatrix}, i = 1, 2, \dots, n$$

where  $\lambda'_i$ ,  $i = 1, 2, \dots, n$  are eigenvalues of  $M_{DD}(G) + 2 \text{diag}(d_{u_i})$ .

*Proof.* First, we state some facts from the definition of  $D_2G$  about the degree of the vertices. As we move from  $G$  to  $D_2G$ , we see that degree for each vertex  $u_i$  in  $G$  is double in  $D_2G$  i.e.,  $d_{u_i}$  in  $G$  becomes  $2d_{u_i}(G)$  in  $D_2G$ . Also for any vertex  $v_i$  in  $D_2G$  we get  $d_{v_i} = 2d_{u_i}(G)$ , for  $i = 1, 2, \dots, n$ . Now from the definition of  $D_2G$  for distances we have:

$$\begin{aligned} d_G(u_i, u_j) &= d_{D_2G}(u_i, u_j) \\ d_G(u_i, v_j) &= d_{D_2G}(u_i, v_j) \\ d_G(u_j, u_i) &= d_{D_2G}(u_j, v_i) \\ d_{D_2G}(u_i, v_i) &= 2. \end{aligned}$$

Using all the above facts regarding change in distances and degrees from  $G$  to  $D_2G$ , and suitable labeling of vertices we get the degree distance matrix of  $D_2G$  as:

$$M_{DD}(D_2G) = \begin{bmatrix} 2M_{DD}(G) & 2M_{DD}(G) - 8 \text{diag}(d_{u_i}) \\ 2M_{DD}(G) - 8 \text{diag}(d_{u_i}) & 2M_{DD}(G) \end{bmatrix}$$

for  $i = 1, 2, \dots, n$ , where each block matrix is of order  $n \times n$ ,  $\text{diag}(d_{u_i})$  is a diagonal matrix with diagonal entries as degrees of vertices  $u_i$ .

From Lemma 3.5, the theorem follows.  $\square$

If  $G$  is a  $k$ -regular vertex degree graph then  $D_2G$  is a  $2k$ -regular vertex degree graph. An immediate consequence of Lemma 2.4 and Theorem 3.7 we state our next lemma.

**Lemma 3.9.** *Let  $G$  be connected graph on  $n$  vertices with degree distance spectrum  $\lambda_1 \geq \lambda_2 \geq \dots \geq \lambda_n$ . Then*

$$\text{spec}_{M_{DD}}(D_2G) = \left( \begin{array}{cc} 8k(\lambda_i + 1) & -8k \\ 1 & n \end{array} \right), i = 1, 2, \dots, n$$

#### 4. BOUNDS ON DEGREE DISTANCE SPECTRAL RADIUS

In this section, we give some sharp bounds on  $\rho(M_{DD}(G))$  for a connected graph  $G$  of order  $n$ . We first recall the following lemma which will be used later on.

**Lemma 4.1** ([17]). *Let  $N = (N_{ij})$  be nonnegative irreducible symmetric matrix with  $n \geq 2$  and row sums  $N_1, N_2, \dots, N_n$ . If  $\rho(N)$  is the largest eigenvalue of  $N$ . Then*

$$\sqrt{\frac{\sum_{i=1}^n N_i^2}{n}} \leq \rho(G) \leq \max_{1 \leq i \leq n} \sum_{j=1}^n N_{ij} \sqrt{\frac{N_j}{N_i}}$$

**Theorem 4.2** (Let  $G$  be a connected graph of order  $n \geq 2$  and  $M_{DD}(G)$  be the degree distance matrix of  $G$ . Let  $M_1, M_2, \dots, M_n$  be the row sums of  $M_{DD}(G)$ . Then).

$$(4.1) \quad \sqrt{\frac{\sum_{i=1}^n M_i^2}{n}} \leq \rho(M_{DD}(G)) \leq \max_{1 \leq i \leq n} \sum_{j=1}^n m_{ij} \sqrt{\frac{M_j}{M_i}}.$$

*Proof.* We see from Lemma 4.1 that left and right inequalities in equation (4.1) hold. Now its important to note that  $m_{ij} > 0$  for all  $i \neq j$  and  $m_{ij} = 0$ , when  $i = j$ . Thus for  $n \geq 3$  there does not exist a permutation matrix  $P$  such that

$$P^T M_{DD} P = \begin{pmatrix} 0 & C \\ C^T & 0 \end{pmatrix}$$

It follows that equality holds in (4.1) if and only if  $M_1 = M_2 = \dots = M_n$  i.e., only if  $G$  is a regular graph.  $\square$

In the upcoming theorems, we will focus on lower bounds for  $M_{DD}$  spectral radius for any connected graph  $G$ .

**Theorem 4.3.** *Let  $G$  be a connected graph of order  $n$  and  $\mathbb{D}_1(G)$  be the degree distance index of  $G$ . Then*

$$\rho(G) \geq \frac{2}{n} \mathbb{D}_1(G)$$

*Moreover, equality holds if row sums are equal.*

*Proof.* Let  $x = \frac{1}{n}(1, 1, \dots, 1)^T \in \mathbb{R}^n$  be a unit vector. Then by the Rayleigh quotient we have

$$\rho(G) \geq x^T M_{DD}(G)x = \frac{2}{n} \sum_{i < j} (d_i + d_j) d_{ij}$$

with equality only if  $x$  is the principal eigenvector of  $M_{DD}(G)$ , i.e., the row sum is constant for each row in  $M_{DD}(G)$ .  $\square$

**Theorem 4.4.** *Let  $G$  be a connected graph of order  $n$ . Let  $\delta_1$  and  $\delta_2$  be the minimum and second minimum vertex degree in  $G$ . Then*

$$(4.2) \quad \rho(G) \geq 2\sqrt{\delta_1\delta_2 Tr_i Tr_j}$$

Moreover the equality holds if  $G$  is a vertex degree and transmission regular graph.

*Proof.* Let  $x = (x_1, x_2, \dots, x_n)^T$  be the Perron eigenvector of degree distance matrix of  $G$  corresponding to  $\rho(G)$ . Let

$$x_i = \min_{k \in V(G)} x_k \quad \text{and} \quad x_j = \min_{\substack{k \in V(G) \\ k \neq i}} x_k$$

Now, by eigenvalue equation for  $M_{DD}(G)$  we can write as  $\rho(G)x = M_{DD}(G)x$ . Next we will focus on the components  $x_i$  and  $x_j$  in the eigenvalue equation. So for component  $x_i$  we have

$$\begin{aligned} \rho(G)x_i &= \sum_{k=1}^n (d_i + d_k)d_{ik}x_k \\ &= d_i \sum_{k=1}^n d_{ik}x_k + \sum_{k=1}^n d_k d_{ik}x_k \\ &\geq 2\delta_1 Tr_i x_j \end{aligned}$$

which implies that:

$$(4.3) \quad \rho(G)x_i \geq 2\delta_1 Tr_i x_j$$

Similarly for component  $x_j$  we have

$$\begin{aligned} \rho(G)x_j &= \sum_{k=1}^n (d_j + d_k)d_{jk}x_k \\ &= d_j \sum_{k=1}^n d_{jk}x_k + \sum_{k=1}^n d_k d_{jk}x_k \\ &\geq 2\delta_2 Tr_j x_i \end{aligned}$$

which implies that:

$$(4.4) \quad \rho(G)x_j \geq 2\delta_2 Tr_j x_i$$

Combining the inequalities (4.3) and (4.4), it follows that

$$\rho(G) \geq \sqrt{(2\delta_1 Tr_i)(2\delta_2 Tr_j)} = 2\sqrt{\delta_1\delta_2 Tr_i Tr_j}$$

Suppose equality holds in the above inequality. Then all inequalities in the above arguments must be equalities. Therefore we have  $x_i = x_j$  for all  $j = 1, 2, \dots, n$ . By  $\rho(G)x = M_{DD}(G)x$ , we can deduce that all the row sums are equal, that is,  $G$  is a vertex degree and transmission regular graph.  $\square$

**Theorem 4.5.** *Let  $G$  be a simple connected graph on  $n$  vertices and  $x$  be an eigenvector corresponding to  $\rho(G)$ . Then*

$$(4.5) \quad \rho(G) \geq \sqrt{(d_i Tr_i + T_i^D)(d_j Tr_j + T_j^D)}$$

Moreover, the equality holds if  $G$  is a vertex degree and transmission regular graph.

*Proof.* Let  $x = (x_1, x_2, \dots, x_n)^T$  be the eigenvector corresponding to eigenvalue  $\rho(G)$  of  $M_{DD}(G)$ . Then by the eigenequation,

$$\rho(G)x = M_{DD}(G)x$$

From the  $k$ th equation of the above eigenequation we have,

$$\rho(G)x_k = d_k \sum_{l \in V(G)} d_{kl}x_l + \sum_{l \in V(G)} d_l d_{lk}x_l, \quad k = 1, 2, \dots, n.$$

As  $M_{DD}(G)$  is irreducible and nonnegative, so we have  $x_k > 0$  for all  $k = 1, 2, \dots, n$ . Let the eigencomponents  $x_i$  and  $x_j$  be the minimum and second minimum components of eigenvector  $x$  respectively i.e.,

$$x_i = \min_{k \in V(G)} x_k, \quad x_j = \min_{\substack{k \in V(G) \\ k \neq i}} x_k,$$

$$x_k \geq x_j \geq x_i > 0.$$

For vertex  $v_i \in V(G)$  by an eigenequation we have,

$$\begin{aligned} \rho(G)x_i &= d_i \sum_{k=1}^n d_{ik}x_k + \sum_{k=1}^n d_k d_{ik}x_k \\ &\geq d_i \sum_{k=1}^n d_{ik}x_j + \sum_{k=1}^n d_k d_{ik}x_j. \end{aligned}$$

So we have

$$(4.6) \quad \rho(G)x_i \geq (d_i Tr_i + T_i^D)x_j.$$

Now for an eigenequation for  $v_j \in V(G)$ ,

$$\begin{aligned} \rho(G)x_j &= d_j \sum_{k=1}^n d_{jk}x_k + \sum_{k=1}^n d_k d_{jk}x_k \\ &\geq d_j \sum_{k=1}^n d_{jk}x_i + \sum_{k=1}^n d_k d_{jk}x_i \end{aligned}$$

$$(4.7) \quad \rho(G)x_j \geq (d_j Tr_j + T_j^D)x_i.$$

From equations (4.6) and (4.7) we see that the left-hand side of the inequalities are positive, so we can multiply both inequalities and get the quadratic form as,

$$\rho(G)^2 \geq (d_i Tr_i + T_i^D)(d_j Tr_j + T_j^D).$$

Thus,

$$\rho(G) \geq \sqrt{(d_i Tr_i + T_i^D)(d_j Tr_j + T_j^D)},$$

which is the required result.

Suppose equality holds in the above inequality. Then all inequalities in the above arguments must be equalities. Therefore we have  $x_i = x_j$  for all  $j = 1, 2, \dots, n$ . By  $\rho(G)x = M_{DD}(G)x$  we can deduce that  $G$  is a vertex degree and transmission regular graph.  $\square$

Next, we state some theorems for the sharp upper bounds for the  $M_{DD}$  spectral radius of any connected graph  $G$ .

**Theorem 4.6.** *Let  $G$  be a connected graph of order  $n$ . Then*

$$\rho(G) \leq \sqrt{\frac{2(n-1)}{n}} \mathcal{S}.$$

where  $\mathcal{S} = \sum_{i < j} ((d_i + d_j)d_{ij})^2$ . Moreover, equality holds if and only if  $G$  is a complete graph.

*Proof.* As  $\rho(G) = \lambda_1(G)$  is the maximum degree distance matrix eigenvalue, so from Lemma 2.2 we see that

$$\sum_{i=1}^n \lambda_i = 0 \implies \lambda_1 = -\sum_{i=2}^n \lambda_i$$

Now by using the Cauchy–Schwarz inequality we get,

$$\begin{aligned} \lambda_1^2 &\leq \left( \sum_{i=2}^n \lambda_i \right)^2 \\ &\leq (n-1) \sum_{i=2}^n \lambda_i^2 \\ &= (n-1) \left[ 2 \sum_{i < j} ((d_i + d_j)d_{ij})^2 - \lambda_1^2 \right], \end{aligned}$$

So from the above inequality we get,

$$n\lambda_1^2 \leq 2(n-1) \sum_{i < j} ((d_i + d_j)d_{ij})^2$$

Hence we have,

$$\rho(G) \leq \sqrt{\frac{2(n-1)}{n}} \mathcal{S}.$$

If the equality holds in the above inequality, then  $\lambda_2 = \dots = \lambda_n$  and  $M_{DD}(G)$  has exactly two distinct eigenvalues. Obviously if  $G = K_n$  then the equality holds.  $\square$

**Theorem 4.7.** *Let  $G$  be a simple connected graph with  $n$  vertices and  $x$  be the eigenvector corresponding to  $\rho(G)$ . Then*

$$(4.8) \quad \rho(G) \leq \max_{1 \leq u \neq w \leq n} \frac{\beta + \sqrt{4(d_u + d_w)(d_u Tr_u + T_u^D)d_{uw} + \beta^2}}{2}$$

where  $\beta = d_w Tr_w + T_w^D - (d_u + d_w)d_{wu}$ . Moreover, equality holds if  $G$  is a vertex degree and transmission regular graph.

*Proof.* Let  $x = (x_1, x_2, \dots, x_n)^T$  be the degree distance Perron vector of  $G$  corresponding to  $\rho(G)$ . Let one eigencomponent  $x_u$  equal 1 and other components are less than or equal to 1 i.e.,  $x_u = 1$  and  $0 \leq x_v \leq 1$  for all  $x_v$ . Let  $x_w = \max(x_v | v \neq u)$ . So by the  $M_{DD}$ -eigenequation:

$$\begin{aligned} \rho(G)x_u &= d_u \sum_{v=1}^n d_{uv}x_v + \sum_{v=1}^n d_v d_{uv}x_v \\ &\leq d_u \sum_{v=1}^n d_{uv}x_w + \sum_{v=1}^n d_v d_{uv}x_w. \end{aligned}$$

$$(4.9) \quad \rho(G)x_u \leq (d_u Tr_u + T_u^D)x_w.$$

Similarly, using the degree distance eigenequation corresponding to  $x_w$ ,

$$\rho(G)x_w = d_w \sum_{v=1}^n d_{wv}x_v + \sum_{v=1}^n d_v d_{wv}x_v$$

Simplifying the above equation by adding and subtracting  $d_w d_{wu}x_w$  and  $d_u d_{u,w}x_w$ , we have

$$\begin{aligned} \rho(G) &= d_w d_{wu}x_u + \left( d_w d_{wu}x_w + d_w \sum_{v \neq u} d_{wv}x_v \right) - d_w d_{wu}x_w \\ &\quad + d_u d_{wu}x_u + \left( d_u d_{wu}x_w + \sum_{v \neq u} d_v d_{wv}x_v \right) - d_u d_{wu}x_w. \end{aligned}$$

Since  $x_w = \max(x_v | v \neq u)$ ,

$$(4.10) \quad \rho(G)x_w \leq (d_u + d_w)d_{wu}x_u - (d_u + d_w)d_{wu}x_w + d_w Tr_w x_w + T_w^D x_w.$$

Now, multiplying both sides of the inequality (4.10) with  $\rho(G)$  we get the quadratic form as,

$$\rho(G)^2 x_w \leq (d_u + d_w)d_{wu}\rho(G)x_u + (d_w Tr_w + T_w^D - (d_u + d_w)d_{wu}\rho(G))x_w.$$

Now substituting equation (4.9) i.e.,  $\rho(G)x_u \leq (d_u Tr_u + T_u^D)x_w$  in the above inequality, the quadratic form becomes easier to simplify as,

$$\rho(G)^2 - (d_w Tr_w + T_w^D - (d_u + d_w)d_{wu}) \rho(G) - (d_u + d_w)(d_u Tr_u + T_u^D)d_{uw} \leq 0.$$

Thus we get the bound (4.8),

$$\rho(G) \leq \max_{1 \leq u \neq w \leq n} \frac{\beta + \sqrt{4(d_u + d_w)(d_u Tr_u + T_u^D)d_{uw} + \beta^2}}{2}$$

where  $\beta = d_w Tr_w + T_w^D - (d_u + d_w)d_{wu}$ .

Suppose equality occurs in equation (4.8), then  $x$  is an eigenvector of  $\rho(G)$  with  $x_u = x_w$  for all  $w = 1, 2, \dots, n$ . This concludes that all the row sums of  $M_{DD}(G)$  are the same and  $G$  is a vertex degree and transmission regular graph.  $\square$

**Theorem 4.8.** *Let  $G$  be a connected graph of order  $n$ . Let  $\Delta_1$  and  $\Delta_2$  be the maximum and second maximum degree in  $G$ . Then*

$$(4.11) \quad \rho(G) \leq 2\sqrt{\Delta_1 \Delta_2 Tr_i Tr_j}$$

*Moreover the equality holds if  $G$  is a vertex degree and transmission regular graph.*

*Proof.* Let  $x = (x_1, x_2, \dots, x_n)^T$  be the Perron eigenvector of the degree distance matrix of  $G$  corresponding to  $\rho(G)$ . Let

$$x_i = \max_{k \in V(G)} x_k \quad x_j = \max_{\substack{k \in V(G) \\ k \neq i}} x_k.$$

Now, by eigenvalue equation for  $M_{DD}(G)$  we can write as  $\rho(G)x = M_{DD}(G)x$ . Next we will focus on the components  $x_i$  and  $x_j$  in the eigenvalue equation. So for component  $x_i$  we have

$$\begin{aligned} \rho(G)x_i &= \sum_{k=1}^n (d_i + d_k)d_{ik}x_k \\ &= d_i \sum_{k=1}^n d_{ik}x_k + \sum_{k=1}^n d_k d_{ik}x_k \\ &\leq 2\Delta_1 Tr_i x_j \end{aligned}$$

which implies that:

$$(4.12) \quad \rho(G)x_i \leq 2\Delta_1 Tr_i x_j.$$

Similarly for component  $x_j$  we have

$$\begin{aligned} \rho(G)x_j &= \sum_{k=1}^n (d_j + d_k)d_{jk}x_k \\ &= d_j \sum_{k=1}^n d_{jk}x_k + \sum_{k=1}^n d_k d_{jk}x_k \\ &\leq 2\Delta_2 Tr_j x_i \end{aligned}$$

which implies that:

$$(4.13) \quad \rho(G)x_j \leq 2\Delta_2 Tr_j x_i.$$

Now, by combining the inequalities (4.12) and (4.13), it follows that

$$\rho(G) \leq \sqrt{(2\Delta_1 Tr_i)(2\Delta_2 Tr_j)} = 2\sqrt{\Delta_1 \Delta_2 Tr_i Tr_j}.$$

Suppose equality holds in the above inequality. Then all inequalities in the above arguments must be equalities. Therefore we have  $x_i = x_j$  for all  $j = 1, 2, \dots, n$ . By  $\rho(G)x = M_{DD}(G)x$ , we can deduce that all the row sums are equal, that is,  $G$  is a vertex degree and transmission regular graph.  $\square$

### 5. DISCUSSION ON THE BOUNDS FOR $\rho(G)$

This section is dedicated to a brief discussion on the bounds for degree distance spectral radius and we will compare different bounds discussed in the paper to the exact degree distance spectral radius of certain graphs (see Figure 2). Let  $G_1, G_2, G_3, G_4, G_5$  and  $G_6$  be connected graphs as shown in Figure 2. We see that  $G_6 = C_6$  is a vertex degree and transmission regular graph, where each vertex is of degree 2 and transmission 9.

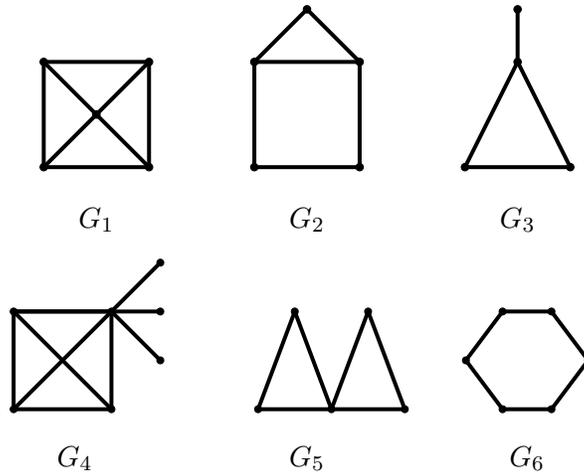


Figure 2: Example of simple connected graphs.

In a sequential way as in the paper, we first depict the lower bounds for  $\rho(G)$  as discussed in Theorems 4.3, 4.4 and 4.5 for graphs  $G_1, G_2, G_3, G_4, G_5$ , and  $G_6$  in Table 1. From Table 1, we can observe that for  $G_6 = C_6$  the equality condition holds for each bound as  $G_6$  is a vertex degree and transmission regular graph.

In the following Table 2, we depict the upper bounds up to three decimal places for Theorems 4.6, 4.7 and 4.8.

	$G_1$	$G_2$	$G_3$	$G_4$	$G_5$	$G_6$
$\rho(G)$	30.439	26.406	15.026	43.083	26.620	36
Theorem 4.3	30.400	26.400	15.000	42.857	25.600	36
Theorem 4.4	26.832	24.000	12.649	34.467	24.000	36
Theorem 4.5	29.462	26.000	14.491	41.893	24.979	36

TABLE 1. Table of  $\rho(G_i)$  for  $i = 1, 2, \dots, 6$ .

	$G_1$	$G_2$	$G_3$	$G_4$	$G_5$	$G_6$
$\rho(G)$	30.439	26.406	15.026	43.083	25.620	36
Theorem 4.6	31.699	27.712	15.199	43.857	26.290	38.987
Theorem 4.7	36.670	27.769	17.489	44.078	25.621	36
Theorem 4.8	30.984	26.832	16.970	62.354	27.712	36

TABLE 2. Table of  $\rho(G_i)$  for  $i = 1, 2, \dots, 6$ .

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