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Further Results on the Largest Eigenvalues of the Distance Matrix and Some Distance–Based Matrices of Connected (Molecular) Graphs

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Further Results on the Largest Eigenvalues of the Distance Matrix and Some Distance–Based Matrices of Connected (Molecular) Graphs

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Abstract

Motivation. Our aim in this report was to detect the upper and lower bounds for the largest eigenvalue of the distance matrix of a connected (molecular) graph involving the distance sums. In addition, we also wanted to detect the largest eigenvalues of related distance–based matrices such as the detour matrix, the Harary matrix (the reciprocal distance matrix) and the complementary distance matrix.

Method. The methods of graph theory and matrix algebra are used.

Results. The upper and lower bounds for the largest eigenvalues of distance matrix and several related distance–based matrices are established.

Conclusions. The bounds for the largest eigenvalues of the four types of distance matrices of connected (molecular) graphs considered here involve the row sums.

Keywords. Largest eigenvalue; distance matrix; detour matrix; Harary matrix; complementary distance matrix.

Abbreviations and notations

G, connected (molecular) graph	**CD**, complementary distance matrix
D, distance matrix	**B**, nonnegative irreducible matrix
DM, detour matrix	Λ_1, largest eigenvalue of distance matrix
RD, Harary matrix (reciprocal distance matrix)	

1 INTRODUCTION

The distance matrix and related matrices, based on graph–theoretical distances, are rich sources of many graph invariants (topological indices) that have found use in structure–property–activity modeling [1–3]. See [4] for these matrices. We consider simple (molecular) graphs [5]. Let G be a connected graph with vertex set $V(G)=\{v_1, v_2, ..., v_n\}$. The distance matrix **D** of G is an $n \times n$ matrix (d_{ij}) such that d_{ij} is just the distance (*i.e.*, the number of edges of a shortest path) between the vertices v_i and v_j in G [4].

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Let G be a connected (molecular) graph. Since $\mathbf{D}$ is a real symmetric matrix, its eigenvalues are all real. Let $\Lambda_1(G)$ be the largest eigenvalue of $\mathbf{D}$. Balaban *et al.* [6] proposed the use of $\Lambda_1(G)$ as a molecular descriptor. In [6,7], it was successfully used to infer the extent of branching and model the boiling points of alkanes. Zhou [8] provided upper and lower bounds for Λ_1 of a tree. Recently, Zhou and Trinajstić [9] provided various upper and lower bounds and the Nordhaus–Gaddum–type result for Λ_1 of connected graphs.

Now we report the upper and lower bounds for the largest eigenvalue Λ_1 of the distance matrix of a connected (molecular) graph involving the distance sums. In addition, we also report bounds for the largest eigenvalues of related distance–based matrices such as the detour matrix, the Harary matrix (the reciprocal distance matrix) and the complementary distance matrix.

2 BOUNDS

First we need the following lemma.

Lemma 1. [10] Let $\mathbf{B}$ be a nonnegative irreducible matrix with row sums $B_1,\ldots,B_n$. If $\rho(\mathbf{B})$ is the largest eigenvalue of $\mathbf{B}$, then $\min_{1\le i\le n} B_i \le \rho(\mathbf{B}) \le \max_{1\le i\le n} B_i$ with either equality if and only if $B_1 = \cdots = B_n$.

Let G be a connected (molecular) graph with $n \ge 2$ vertices. Let $D_i = \sum_{j=1}^{n} d_{ij}$ be the distance sum of vertex v_i in G. We have shown in [8] that

$$\sqrt{\frac{\sum_{i=1}^{n} D_i^2}{n}} \le \Lambda_1(G) \le \max_{1\le i\le n} \sum_{j=1}^{n} d_{ij}\sqrt{\frac{D_j}{D_i}}$$

with either equality if and only if $D_1 = \cdots = D_n$. This implies that $\min_{1\le i\le n} D_i \le \Lambda_1(G) \le \max_{1\le i\le n} D_i$ with either equality if and only if $D_1 = \cdots = D_n$, which follows also from Lemma 1. In the following we consider graphs whose distance sums are not all equal.

Theorem 1. Let G be a connected (molecular) graph with $n \ge 2$ vertices. Suppose that $D_1 \ge \cdots \ge D_n$ and $D_1 > D_{n-k+1}$, $1 \le k \le n-1$. Then

$$\Lambda_1(G) \le \frac{D_1 - 1}{2} + \sqrt{\frac{(D_1+1)^2}{4} - k(D_1 - D_{n-k+1})} \tag{1}$$

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

Proof. Let $V_1 = \{v_1,...,v_{n-k}\}$ and $V_2 = V(G)\setminus V_1$. Then the distance matrix may be partitioned as

$$\mathbf{D} = \begin{pmatrix} \mathbf{D_{11}} & \mathbf{D_{12}} \\ \mathbf{D_{21}} & \mathbf{D_{22}} \end{pmatrix},$$

where $\mathbf{D_{11}}$ is an $(n-k)\times(n-k)$ matrix. Let

$$\mathbf{U} = \begin{pmatrix} \frac{1}{x}\mathbf{I}_{n-k} & \mathbf{0} \\ \mathbf{0} & \mathbf{I}_k \end{pmatrix}$$

for $0 < x < 1$ (to be determined) and $\mathbf{B} = \mathbf{U}^{-1}\mathbf{DU}$, where $\mathbf{I}_s$ the $s\times s$ unit matrix. Then

$$\mathbf{B} = \begin{pmatrix} \mathbf{D_{11}} & x\mathbf{D_{12}} \\ \frac{1}{x}\mathbf{D_{21}} & \mathbf{D_{22}} \end{pmatrix}$$

is a nonnegative irreducible matrix that has the same spectrum as $\mathbf{D}$. We consider the row sums of $\mathbf{B}$. If $i = 1,...,n-k$, then since $d_{ij} \geq 1$ for $j = n-k+1,...,n$, we have

$$B_i = \sum_{j=1}^{n-k} d_{ij} + x\sum_{j=n-k+1}^{n} d_{ij} = \sum_{j=1}^{n} d_{ij} + (x-1)\sum_{j=n-k+1}^{n} d_{ij}$$
$$= D_i + (x-1)\sum_{j=n-k+1}^{n} d_{ij} \leq D_i + (x-1)k \leq D_1 + (x-1)k.$$

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

$$B_i = \frac{1}{x}\sum_{j=1}^{n-k} d_{ij} + \sum_{j=n-k+1}^{n} d_{ij} = \frac{1}{x}\sum_{j=1}^{n} d_{ij} + \left(1-\frac{1}{x}\right)\sum_{j=n-k+1}^{n} d_{ij}$$
$$= \frac{1}{x}D_i + \left(1-\frac{1}{x}\right)\sum_{j=n-k+1}^{n} d_{ij} \leq \frac{1}{x}D_i + \left(1-\frac{1}{x}\right)(k-1) \leq \frac{1}{x}D_{n-k+1} + \left(1-\frac{1}{x}\right)(k-1).$$

Let

$$x = \frac{2k-1-D_1+\sqrt{(D_1+1)^2-4k(D_1-D_{n-k+1})}}{2k}.$$

Then $D_1 + (x-1)k = \frac{1}{x}D_{n-k+1} + \left(1-\frac{1}{x}\right)(k-1) = \frac{D_1-1}{2} + \sqrt{\frac{(D_1+1)^2}{4} - k(D_1-D_{n-k+1})}.$ Since $D_1 > D_{n-k+1} \geq D_n \geq n-1 > k-1$, we have $0 < x < 1$. Thus by Lemma 1, we have

$$\Lambda_1(G) \leq \max_{1\leq i\leq n} B_i \leq \frac{D_1-1}{2} + \sqrt{\frac{(D_1+1)^2}{4} - k(D_1-D_{n-k+1})}.$$

This proves (1).

Suppose that equality holds in (1). Then

$$B_1 = \cdots = B_n = D_1 + (x-1)k = \frac{1}{x} D_{n-k+1} + \left(1 - \frac{1}{x}\right)(k-1).$$

Since $B_i = D_1 + (x-1)k$ for $i = 1,...,n-k,$ we have $d_{ij} = 1$ for $i = 1,...,n-k$ and $j = n-k+1,...,n,$ which implies that every vertex in V_1 is adjacent to all vertices in V_2. Since $B_i = \frac{1}{x} D_{n-k+1} + \left(1 - \frac{1}{x}\right)(k-1)$ for $i = n-k+1,...,n,$ we have $d_{ij} = 1$ for $i, j = n-k+1,...,n$ with $j \neq i,$ which implies that V_2 induces a complete subgraph in G. Thus, the degree of every vertex in V_2 is $n-1,$ and then the diameter of G is at most 2. Since $D_1 = \cdots = D_{n-k}$, every vertex in V_1 has the same degree, say s. Moreover, since $D_1 > D_{n-k+1}$, G can not be the complete graph, and then $k, s \leq n-2.$

Conversely, if G is a graph stated in the second part of the theorem, then from the proof above, we have $B_1 = \cdots = B_n$ and thus (1) is an equality. □

Theorem 2. Let G be a connected (molecular) graph with $n \geq 2$ vertices. Suppose that $D_1 \geq \cdots \geq D_n$ and $D_l > D_n$, $1 \leq l \leq n-1.$ Then

$$\Lambda_1(G) > \frac{D_n - 1}{2} + \sqrt{\frac{(D_n+1)^2}{4} + l(D_l - D_n)}.$$

Proof. Let $k = n - l$ and $x = \frac{1}{y}$ ($y > 1,$ to be determined) in the proof of Theorem 1. Then

$$\mathbf{B} = \begin{pmatrix} \mathbf{D_{11}} & \frac{1}{y}\mathbf{D_{12}} \\ y\mathbf{D_{21}} & \mathbf{D_{22}} \end{pmatrix}$$

is a nonnegative irreducible matrix that has the same spectrum as $\mathbf{D}$. If $i = 1,...,l,$ then since $d_{ii} = 0$ and $d_{ij} \geq 1$ for $j = 1,...,l$ with $j \neq i,$ we have

$$B_i = \sum_{j=1}^{l} d_{ij} + \frac{1}{y}\sum_{j=l+1}^{n} d_{ij} = \frac{1}{y} D_i + \left(1 - \frac{1}{y}\right)\sum_{j=1}^{l} d_{ij} \geq \frac{1}{y} D_l + \left(1 - \frac{1}{y}\right)(l-1).$$

If $i = l+1,...,n,$ then since $d_{ij} \geq 1$ for $j = 1,...,l,$ we have

$$B_i = y\sum_{j=1}^{l} d_{ij} + \sum_{j=l+1}^{n} d_{ij} = D_i + (y-1)\sum_{j=1}^{l} d_{ij} \geq D_n + (y-1)l.$$

Let

$$y = \frac{2l - 1 - D_n + \sqrt{(D_n+1)^2 + 4l(D_l - D_n)}}{2l}.$$

Then $\frac{1}{y} D_l + \left(1 - \frac{1}{y}\right)(l-1) = D_n + (y-1)l = \frac{D_n - 1}{2} + \sqrt{\frac{(D_n+1)^2}{4} + l(D_l - D_n)}.$ Since $D_l > D_n$, we have $y > 1$. Thus by Lemma 1, we have

$$\Lambda_1(G) \geq \min_{1 \leq i \leq n} B_i \geq \frac{D_n - 1}{2} + \sqrt{\frac{(D_n + 1)^2}{4} + l(D_l - D_n)} .$$

Suppose that $\Lambda_1(G) = \frac{D_n - 1}{2} + \sqrt{\frac{(D_n + 1)^2}{4} + l(D_l - D_n)}$. Then

$$B_1 = \cdots = B_n = \frac{1}{y} D_l + \left(1 - \frac{1}{y}\right)(l - 1) = D_n + (y - 1)l .$$

Since $B_i = \frac{1}{y} D_l + \left(1 - \frac{1}{y}\right)(l - 1)$ for $i = 1, \ldots, l,$ we have $d_{ij} = 1$ for $i, j = 1, \ldots, l$ with $j \neq i,$ which implies that V_1 induces a complete subgraph in G. Since $B_i = D_n + (y - 1)l$ for $i = l + 1, \ldots, n,$ we have $d_{ij} = 1$ for $i = l + 1, \ldots, n$ and $j = 1, \ldots, l,$ which implies that every vertex in V_2 is adjacent to all vertices in V_1. Thus the degree of every vertex in V_1 is $n - 1,$ and then $D_1 = \cdots = D_l = n - 1$, which is a contradiction to the assumption that $D_l > D_n$. □

Remark 1. Similar techniques have been used to derive upper bound for the spectral radius of (the adjacency matrix of) a graph in [11].

Remark 2. Let G be a connected (molecular) graph with n vertices, and let $S(G)$ be the sum of the squares of the distances between all unordered pairs of vertices in G. Recently, we showed in [9] that

$$\Lambda_1(G) \leq \sqrt{\frac{2(n - 1)}{n} S(G)}$$

with equality if and only if G is the complete graph (where the condition that the distance matrix has exactly one positive eigenvalue may be dropped). Thus, for $n \geq 3,$ we have $\Lambda_1(G) < \sqrt{\frac{(n + 1)n(n - 1)^2}{6}},$ and if $n \geq 4$ and the complement $\overline{G}$ of G is also connected, then $\Lambda_1(G) + \Lambda_1(\overline{G}) < \sqrt{\frac{(n + 1)n(n - 1)^2}{6}} + 2n - 3.$

Now we turn to some other distance–related matrices. The detour matrix $\mathbf{DM}$ of a connected (molecular) graph G with n vertices is an $n \times n$ matrix (dm_{ij}) such that dm_{ij} is equal to the length of the longest distance between vertices v_i and v_j if $i \neq j,$ and 0 otherwise [4,12–14]. Note that $\mathbf{DM} = \mathbf{D}$ if G is a tree. Let $M_i = \sum_{j=1}^{n} dm_{ij}$. Let $\Gamma_1(G)$ be the largest eigenvalue of $\mathbf{DM}$.

Let G be a connected (molecular) graph with n vertices. Then $dm_{ij} \leq n - 1$ with equality if and only if there is a path of length $n - 1$ between vertices v_i and v_j. By Lemma 1, $\Gamma_1(G) \leq (n - 1)^2$ with equality if and only if all row sums of $\mathbf{DM}$ are equal to $(n - 1)^2$, or equivalently, there is a path of length $n-1$ between every pair of distinct vertices of G, *i.e.*, G is a Hamilton–connected graph.

Note that $dm_{ij} \geq 1$ with equality if and only if v_i and v_j are adjacent and the edge v_iv_j lies outside any cycle for $i, j = 1,...,n$ with $i \neq j$. Let $V(G) = V_1 \cup V_2$ be a partition of $V(G)$. If $dm_{ij} = 1$ for any $v_i \in V_1$ and $v_j \in V_2$ and for any $v_i, v_j \in V_2$ with $v_i \neq v_j$, then every vertex in V_1 is adjacent to all vertices in V_2 and V_2 induces a complete subgraph in G, and thus $|V_2| = 1$ and V_1 is an independent set in G, *i.e.*, G is the star. Similarly to Theorems 1 and 2, we have:

Theorem 3. Let G be a connected (molecular) graph with n vertices. Suppose that $M_1 \geq \cdots \geq M_n$.

(*i*) If $M_1 > M_{n-k+1}$, $1 \leq k \leq n-1$, then

$$\Gamma_1(G) \leq \frac{M_1 - 1}{2} + \sqrt{\frac{(M_1+1)^2}{4} - k(M_1 - M_{n-k+1})}$$

with equality if and only if $k = 1$ and G is the star.

(*ii*) If $M_l > M_n$, $1 \leq l \leq n-1$, then

$$\Gamma_1(G) > \frac{M_n - 1}{2} + \sqrt{\frac{(M_n+1)^2}{4} + l(M_l - M_n)} \, .$$

Let G be a connected (molecular) graph with n vertices. The reciprocal distance matrix **RD** of G, also called the Harary matrix, is an $n \times n$ matrix (r_{ij}) such that $r_{ij} = \frac{1}{d_{ij}}$ if $i \neq j$, and 0 otherwise [4,15,16]. Let $R_i = \sum_{j=1}^{n} r_{ij}$. Let $\lambda_1(G)$ be the largest eigenvalue of **RD**, see [17]. Note that $r_{ij} \leq 1$ with equality if and only if v_i and v_j are adjacent for $i, j = 1,...,n$ with $i \neq j$. Similarly, we have:

Theorem 4. Let G be a connected (molecular) graph with n vertices. Suppose that $R_1 \geq \cdots \geq R_n$.

(*i*) If $R_1 > R_{l+1}$, where $1 \leq l \leq n-1$, then

$$\lambda_1(G) \leq \frac{R_{l+1} - 1}{2} + \sqrt{\frac{(R_{l+1}+1)^2}{4} + l(R_1 - R_{l+1})}$$

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

(*ii*) If $R_{n-k} > R_n > k-1$, where $1 \leq k \leq n-1$, then

$$\lambda_1(G) > \frac{R_{n-k} - 1}{2} + \sqrt{\frac{(R_{n-k}+1)^2}{4} - k(R_{n-k} - R_n)} \, .$$

Proof. (*i*) Let $V_1 = \{v_1,...,v_l\}$ and $V_2 = V(G) \setminus V_1$. Then the reciprocal distance matrix may be partitioned as

$$\mathbf{RD} = \begin{pmatrix} \mathbf{RD_{11}} & \mathbf{RD_{12}} \\ \mathbf{RD_{21}} & \mathbf{RD_{22}} \end{pmatrix},$$

where $\mathbf{RD_{11}}$ is an $l \times l$ matrix. For $y > 1$ (to be determined),

$$\mathbf{B} = \begin{pmatrix} \mathbf{RD_{11}} & \frac{1}{y}\mathbf{RD_{12}} \\ y\mathbf{RD_{21}} & \mathbf{RD_{22}} \end{pmatrix}$$

is a nonnegative irreducible matrix that has the same spectrum as **RD**. If $i = 1,...,l,$ then since $r_{ii} = 0$ and $r_{ij} \le 1$ for $j = 1,...,l$ with $j \ne i,$ we have

$$B_i = \sum_{j=1}^{l} r_{ij} + \frac{1}{y}\sum_{j=l+1}^{n} r_{ij} = \frac{1}{y}R_i + \left(1 - \frac{1}{y}\right)\sum_{j=1}^{l} r_{ij} \le \frac{1}{y}R_1 + \left(1 - \frac{1}{y}\right)(l-1).$$

If $i = l+1,...,n,$ then since $r_{ij} \le 1$ for $j = 1,...,l,$ we have

$$B_i = y\sum_{j=1}^{l} r_{ij} + \sum_{j=l+1}^{n} r_{ij} = R_i + (y-1)\sum_{j=1}^{l} r_{ij} \le R_{l+1} + (y-1)l.$$

Let

$$y = \frac{2l - 1 - R_{l+1} + \sqrt{(R_{l+1}+1)^2 + 4l(R_1 - R_{l+1})}}{2l}.$$

Then $\frac{1}{y}R_1 + \left(1 - \frac{1}{y}\right)(l-1) = R_{l+1} + (y-1)l = \frac{R_{l+1}-1}{2} + \sqrt{\frac{(R_{l+1}+1)^2}{4} + l(R_1 - R_{l+1})}.$ Since $R_1 > R_{l+1},$ we have $y > 1.$ Thus by Lemma 1, we have

$$\lambda_1(G) \le \max_{1 \le i \le n} B_i \le \frac{R_{l+1}-1}{2} + \sqrt{\frac{(R_{l+1}+1)^2}{4} + l(R_1 - R_{l+1})}.$$

Suppose that $\lambda_1(G) = \frac{R_{l+1}-1}{2} + \sqrt{\frac{(R_{l+1}+1)^2}{4} + l(R_1 - R_{l+1})}$. Then

$$B_1 = \cdots = B_n = \frac{1}{y}R_1 + \left(1 - \frac{1}{y}\right)(l-1) = R_{l+1} + (y-1)l.$$

Thus, $r_{ij} = 1$ for $i, j = 1,...,l$ with $j \ne i,$ and for $i = l+1,...,n$ and $j = 1,...,l,$ which implies that every vertex in V_1 is adjacent to all other vertices of $G,$ and then the diameter of G is $2.$ Since $R_{l+1} = \cdots = R_n$ and $R_1 > R_{l+1},$ every vertex in V_2 has the same degree, say $s,$ and $k, s \le n-2.$

(*ii*) Let $l = n - k$ and $y = \frac{1}{x}$ ($0 < x < 1,$ to be determined) in the proof above. If $i = 1,...,n-k,$ then since $r_{ij} \le 1$ for $j = n-k+1,...,n,$ we have

$$B_i = \sum_{j=1}^{n-k} r_{ij} + x \sum_{j=n-k+1}^{n} r_{ij} = R_i + (x-1)\sum_{j=n-k+1}^{n} r_{ij} \ge R_{n-k} + (x-1)k\ .$$

If $i = n-k+1,\ldots,n,$ then $r_{ii} = 0$ and $r_{ij} \le 1$ for $j = n-k+1,\ldots,n$ with $j \ne i,$ we have

$$B_i = \frac{1}{x}\sum_{j=1}^{n-k} r_{ij} + \sum_{j=n-k+1}^{n} r_{ij} = \frac{1}{x}R_i + \left(1-\frac{1}{x}\right)\sum_{j=n-k+1}^{n} r_{ij} \ge \frac{1}{x}R_n + \left(1-\frac{1}{x}\right)(k-1)\ .$$

Let

$$x = \frac{2k-1-R_{n-k} + \sqrt{(R_{n-k}+1)^2 - 4k(R_{n-k}-R_n)}}{2k}\ .$$

Then $R_{n-k} + (x-1)k = \frac{1}{x}R_n + \left(1-\frac{1}{x}\right)(k-1) = \frac{R_{n-k}-1}{2} + \sqrt{\frac{(R_{n-k}+1)^2}{4} - k(R_{n-k}-R_n)}.$ Since $R_{n-k} \ge R_n > k-1,$ we have $0 < x < 1$. Thus by Lemma 1, we have

$$\lambda_1(G) \ge \min_{1\le i\le n} B_i \ge \frac{R_{n-k}-1}{2} + \sqrt{\frac{(R_{n-k}+1)^2}{4} - k(R_{n-k}-R_n)}\ .$$

If $\lambda_1(G) = \frac{R_{n-k}-1}{2} + \sqrt{\frac{(R_{n-k}+1)^2}{4} - k(R_{n-k}-R_n)},$ then

$$B_1 = \cdots = B_n = R_{n-k} + (x-1)k = \frac{1}{x}R_n + \left(1-\frac{1}{x}\right)(k-1)\ ,$$

and thus $d_{ij} = 1$ for $i = 1,\ldots,n-k$ and $j = n-k+1,\ldots,n,$ and for $i, j = n-k+1,\ldots,n$ with $j \ne i,$ which implies that every vertex in V_1 is adjacent to all other vertices of G, and we have $R_{n-k+1} = \cdots = R_n = n-1,$ contradicting the assumption that $R_{n-k} > R_n$. □

A variant of the Harary matrix is derived from the Harary matrix by replacing its elements $\frac{1}{d_{ij}}$ with $\frac{1}{d_{ij}^2}$ if $i \ne j,$ see [18]. From the proof above, similar result holds for this matrix.

Let G be a connected (molecular) graph with n vertices. The complementary distance matrix **CD** of G is an $n \times n$ matrix (c_{ij}) such that $c_{ij} = 1 + \Delta - d_{ij}$ if $i \ne j,$ and 0 otherwise, where Δ is the diameter of G [4,19,20]. Let $C_i = \sum_{j=1}^{n} c_{ij}$. Let $\mu_1(G)$ be the largest eigenvalue of **CD**. By Lemma 1, $\mu_1(G) \ge n-1$ with equality if and only if G is the complete graph. Note that $c_{ij} \ge 1$ with equality if and only if d_{ij} is equal to the diameter of G for $i, j = 1,\ldots,n$ with $i \ne j$. For any partition of the vertex set $V(G) = V_1 \cup V_2,$ there is at least one edge connecting a vertex, say v_i in V_1 and a vertex, say v_j in $V_2,$ and so if $c_{ij} = 1$ then the diameter of G is one, *i.e.*, G is a complete graph, for which **CD** has equal row sums. Similarly, we have:

Theorem 5. Let G be a connected (molecular) graph with n vertices. Suppose that $C_1 \geq \cdots \geq C_n$.

(*i*) If $C_1 > C_{n-k+1}$, $1 \leq k \leq n-1$, then

$$\mu_1(G) < \frac{C_1 - 1}{2} + \sqrt{\frac{(C_1+1)^2}{4} - k(C_1 - C_{n-k+1})}\,.$$

(*ii*) If $C_l > C_n$, $1 \leq l \leq n-1$, then

$$\mu_1(G) > \frac{C_n - 1}{2} + \sqrt{\frac{(C_n+1)^2}{4} + l(C_l - C_n)}\,.$$

3 CONCLUSIONS

The distance matrix of a connected graph is a mathematical object that found considerable applications in chemistry. However, it is much less studied than the adjacency matrix, *e.g.*, [21]. One of the interesting problems to study is the spectra of distance matrix and various related matrices based on graph–theoretical distances. In this report we presented our study on the bounds of the largest eigenvalues of four distance–based matrices, that is, the standard distance matrix, the detour matrix, the Harary matrix or the reciprocal distance matrix and the complementary distance matrix. The result of our analysis is the upper and lower bounds of the studied matrices depend on the graph structures in terms of row sums.

The Editor and the reviewers raised the following question, that is, is it possible the present analysis to apply to other matrices derived from the distance matrix such as the reverse–Wiener matrix **RW** [4,22] and for the distance matrix of the edge–weighted graphs [2–5]? Our answers on these questions are as follows.

Using the method presented in this report, we have obtained the trivial result for **RW**: the largest eigenvalue is placed between the minimum and maximum row sums of **RW**. But, if the graph–diameter is used we may obtain different bounds.

It is possible to extend the present approach to edge–weighted molecular graphs. For example, for connected (molecular) edge–weighted graph G, the edge–weighted distance matrix ${}^{ew}\mathbf{D}$ is defined as the $n \times n$ matrix such that its (i,j)–entry is the minimum–sum of edge–weights along the path between vertices v_i and v_j in G if $i \neq j$, and 0 otherwise. Let G be a connected (molecular) edge–weighted graph with $n \geq 2$ vertices. Suppose that the row sums of ${}^{ew}\mathbf{D}$ satisfy ${}^{ew}D_1 \geq \cdots \geq {}^{ew}D_n$ and ${}^{ew}D_1 > {}^{ew}D_{n-k+1}$, $1 \leq k \leq n-1$. If the minimum weight is $r > 0$, then (1) may be extended as:

$$\Lambda_1(G) \leq \frac{D_1 - r}{2} + \sqrt{\frac{(D_1+r)^2}{4} - kr(D_1 - D_{n-k+1})}\,.$$

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4 REFERENCES

[1] Z. Mihalić, D. Veljan, D. Amić, S. Nikolić, D. Plavšić, and N. Trinajstić, The distance matrix in chemistry, *J. Math. Chem.* **1992**, *11*, 223–258.
[2] J. Devillers and A. T. Balaban, Eds., *Topological Indices and Related Descriptors in QSAR and QSPR*, Gordon and Breach, Amsterdam, 1999.
[3] R. Todeschini and V. Consonni, *Handbook of Molecular Descriptors*, Wiley–VCH, Weinheim, 2000.
[4] D. Janežič, A. Miličević, S. Nikolić, N. Trinajstić, *Graph Theoretical Matrices in Chemistry*, Mathematical Chemistry Monographs No. 3, University of Kragujevac, Kragujevac, 2007, pp. 5–50.
[5] N. Trinajstić, *Chemical Graph Theory*, 2nd revised ed., CRC press, Boca Raton, 1992.
[6] A. T. Balaban, D. Ciubotariu, and M. Medeleanu, Topological indices and real number vertex invariants based on graph eigenvalues or eigenvectors, *J. Chem. Inf. Comput. Sci.* **1991**, *31*, 517–523.
[7] I. Gutman and M. Medeleanu, On the structure–dependence of the largest eigenvalue of the distance matrix of an alkane, *Indian J. Chem. A* **1998**, *37*, 569–673.
[8] B. Zhou, On the largest eigenvalue of the distance matrix of a tree, *MATCH Commun. Math. Comput. Chem.* **2007**, *58*, 657–662.
[9] B. Zhou and N. Trinajstić, On the largest eigenvalue of the distance matrix of a connected graph, *Chem. Phys. Lett.* **2007**, *447*, 384–387.
[10] A. Berman and R. J. Plemmons, *Nonnegative Matrices in the Mathematical Sciences*, SIAM, Philadelphia, 1994.
[11] J. Shu and Y. Wu, Sharp upper bounds on the spectral radius of graphs, *Lin. Algebra Appl.* **2004**, *377*, 241–248.
[12] O. Ivanciuc and A. T. Balaban, Design of topological indices. Part 8. Path matrices and derived molecular graph invariants, *MATCH Commun. Math. Comput. Chem.* **1994**, *30*, 141–152.
[13] N. Trinajstić, S. Nikolić, and B. Lučić, The detour matrix in chemistry, *J. Chem. Inf. Comput. Sci.* **1997**, *37*, 631–638.
[14] S. Nikolić, N. Trinajstić, and Z. Mihalić, The detour matrix and the detour index; in: *Topological Indices and Related Descriptors in QSAR and QSPR*, Eds. J. Devillers and A. T. Balaban, Gordon and Breach, Amsterdam, 1999, pp. 279–306.
[15] D. Plavšić, S. Nikolić, N. Trinajstić, and Z. Mihalić, On the Harary index for the characterization of chemical graphs, *J. Math. Chem.* **1993**, *12*, 235–250.
[16] O. Ivanciuc, T. S. Balaban, and A. T. Balaban, Reciprocal distance matrix, related local vertex invariants and topological indices, *J. Math. Chem.* **1993**, *12*, 309–318.
[17] B. Zhou and N. Trinajstić, On the maximum eigenvalues of the reciprocal distance matrix and the reverse Wiener matrix, *Int. J. Quantum Chem.*, in press.
[18] Z. Mihalić and N. Trinajstić, A graph–theoretical apporach to structure–property relationships, *J. Chem. Educ.* **1992**, *69*, 701–712.
[19] O. Ivanciuc, QSAR comparative study of Wiener descriptors for weighted molecular graphs, *J. Chem. Inf. Comput. Sci.* **2000**, *40*, 1412–1422.
[20] O. Ivanciuc, T. Ivanciuc, and A. T. Balaban, The complementary distance matrix, a new molecular graph metric, *ACH–Models Chem.* **2000**, *137*, 57–82.
[21] D. M. Cvetković, M. Doob, and H. Sachs, *Spectra of Graphs – Theory and Application*, 3rd ed., Johann Ambrosius Barth, Heidelberg, 1995.
[22] *e.g.*, O. Ivanciuc, Graph theory in chemistry; in: *Handbook on Cheminformatics*, Ed. J. Gasteiger, Wiley–VCH, 2003, pp. 103–138.