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Maximum eigenvalue of the reciprocal distance matrix

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Abstract In this paper, we obtain the lower and upper bounds of the maximum eigenvalue of the reciprocal distance matrix of a connected (molecular) graph. We also give the Nordhaus-Gaddum-type result for the maximum eigenvalue.

Keywords Molecular graph · Reciprocal distance matrix · Maximum eigenvalue · Diameter · Lower bound · Upper bound

1 Introduction

Since the distance matrix and related matrices, based on graph-theoretical distances [1], are rich sources of many graph invariants (topological indices) that have found use in structure-property-activity modeling [2–4], it is of interest to study spectra and polynomials of these matrices [5–7].

Let $G = (V, E)$ be a simple connected graph with vertex set $V(G) = \{v_1, v_2, \ldots, v_n\}$ and edge set $E(G)$, where $|V(G)| = n$ and $|E(G)| = m$. Let $\overline{G}$ be the complement of G. For $v_i \in V(G)$, $\Gamma(v_i)$ denotes the set of its (first) neighbors in G and the degree of v_i is $d_i = |\Gamma(v_i)|$. The minimum vertex degree is denoted by δ and the maximum by Δ. The average of the degrees of the vertices adjacent to v_i is denoted by μ_i. The diameter of a graph is the maximum distance between any two vertices of G. Let d be the diameter of G. The distance matrix D of G is an $n \times n$ matrix $(d_{i,j})$ such that $d_{i,j}$ is just the distance (i.e., the number of edges of a shortest path) between the vertices v_i and v_j in G [1]. The reciprocal distance matrix RD of G, also called the Harary matrix [1], is an $n \times n$ matrix $(RD_{i,j})$ such that [8, 9].

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$$RD_{i,j} = \begin{cases} \frac{1}{d_{i,j}} & \text{if } i \neq j, \\ 0 & \text{if } i = j. \end{cases}$$

Since RD is a real symmetric matrix, its all eigenvalues are real. Let $\lambda(G)$ be the maximum eigenvalue of RD. Ivanciuc et al. [10] have shown that $\lambda(G)$ is able to produce fair QSPR models for the boiling points, molar heat capacities, vaporization enthalpies, refractive indices and densities for $C_6 - C_{10}$ alkanes. The maximum eigenvalues of various matrices has recently attracted attention of mathematical chemists [11–16]. The lower and upper bounds of the maximum eigenvalue of the reciprocal distance matrix in terms of the number of vertices and/or the number of edges, and the Nordhaus-Gaddum-type result for the maximum eigenvalue of the reciprocal distance matrix were obtained in [17].

In this paper we report lower and upper bounds for the maximum eigenvalue of the reciprocal distance matrix and also provide the Nordhaus-Gaddum-type results for maximum eigenvalue. Lastly, we compare our results with the previous results given by Zhou and Trinajsti [17].

2 Spectral radius of reciprocal distance matrix

Zhou et al. [17] gave the following lower bound for $\lambda(G)$ in terms of n, m and d:

Lemma 2.1 *Let G be a connected graph with $n \geq 2$ vertices, m edges and diameter d. Then*

$$\lambda(G) \geq \frac{2m}{n} + \frac{1}{d}\left(n - 1 - \frac{2m}{n}\right), \tag{1}$$

with equality holds if and only if G is a complete graph K_n or G is a regular graph of diameter 2.

Lemma 2.2 [18] *Let $B = (b_{i,j})$ be an $n \times n$ irreducible nonnegative matrix with spectral radius $\lambda(B)$, and let $R_i(B)$ be the ith row sum of B, i.e., $R_i(B) = \sum_{j=1}^{n} b_{i,j}$. Then*

$$\min\{R_i(B) : 1 \leq i \leq n\} \leq \lambda(B) \leq \max\{R_i(B) : 1 \leq i \leq n\}. \tag{2}$$

Moreover, if the row sums of B are not all equal, then the both inequalities in (2) are strict.

Lemma 2.3 (Rayleigh-Ritz) [19] *If A is a symmetric $n \times n$ matrix with eigenvalues $\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_n$ then for any $\mathbf{X} \in R^n$ ($\mathbf{X} \neq \mathbf{0}$),*

$$\mathbf{X}^T A \mathbf{X} \leq \lambda_1 \mathbf{X}^T \mathbf{X}. \tag{3}$$

Equality holds if and only if $\mathbf{X}$ is an eigenvector of A corresponding to the largest eigenvalue λ_1.

Now we give a lower bound for $\lambda(G)$ in terms of the number of vertices n, number of edges m, diameter d and degree sequence $d_1, d_2, \ldots, d_n$.

Theorem 2.4 *Let G be a connected graph with $n \geq 2$ vertices, m edges, and diameter d. Then*

$$\lambda(G) \geq \frac{2m}{n} + \frac{1}{nd}\left(n(n-1) - 2m\right) + \frac{1}{n\Delta^2}\left(\left(1 - \frac{1}{d}\right)\sum_{i=1}^{n} d_i^3 - \frac{4m^2}{d} + \frac{n}{d}M_1(G) - 2\left(1 - \frac{1}{d}\right)M_2(G)\right) \tag{4}$$

where d_i is the degree of vertex v_i, $M_1(G) = \sum_{i=1}^{n} d_i^2$, and $M_2(G) = \sum_{ij\in E(G)} d_i d_j$. Moreover, the equality holds in (4) if and only if G is a complete graph K_n or G is isomorphic to a regular graph of diameter 2.

Proof Let $\mathbf{X} = (x_1, x_2, \ldots, x_n)^T$ be any unit vector. Since the spectral radius of $RD(G)$ and $D(G)^{-1}RD(G)D(G)$ ($D(G)$ is the diagonal matrix whose diagonal elements are the degrees of the vertices of graph G) are same, then by (3), we get

$$\mathbf{X}^T\{D(G)^{-1}RD(G)D(G)\}\mathbf{X} \leq \lambda(G)\mathbf{X}^T\mathbf{X}. \tag{5}$$

Since $\sum_{i=1}^{n} x_i^2 = 1$, from (5), we get

$$\lambda(G) \geq \sum_{i=1}^{n}\sum_{j=1, j\neq i}^{n} \frac{d_j x_i x_j}{d_i d_{i,j}}\,. \tag{6}$$

Since $\mathbf{X}$ is any unit vector, we can assume that $\mathbf{X} = \left(\frac{1}{\sqrt{n}}, \frac{1}{\sqrt{n}}, \cdots, \frac{1}{\sqrt{n}}\right)^T$. From (6), we get

$$\begin{aligned}\lambda(G) &\geq \frac{1}{n}\sum_{i<j}\frac{1}{d_{i,j}}\left(\frac{d_i}{d_j} + \frac{d_j}{d_i}\right) \quad \text{as } d_{i,j} = d_{j,i}\\ &\geq \frac{1}{n}\sum_{ij\in E(G)}\left(\frac{d_i}{d_j} + \frac{d_j}{d_i}\right) + \frac{1}{nd}\sum_{i<j: d_{i,j}\geq 2}\left(\frac{d_i}{d_j} + \frac{d_j}{d_i}\right) \quad \text{as } d \geq d_{i,j}.\end{aligned} \tag{7}$$

Now,

$$\begin{aligned}\sum_{ij\in E(G)}\left(\frac{d_i}{d_j} + \frac{d_j}{d_i}\right) &= 2m + \sum_{ij\in E(G)}\frac{(d_i - d_j)^2}{d_i d_j}\\ &\geq 2m + \frac{1}{\Delta^2}\left(\sum_{ij\in E(G)}(d_i^2 + d_j^2) - 2\sum_{ij\in E(G)} d_i d_j\right)\end{aligned} \tag{8}$$

$$= 2m + \frac{1}{\Delta^2}\left(\sum_{i=1}^{n} d_i^3 - 2M_2(G)\right), \tag{9}$$

and

$$\sum_{i<j:d_{i,j}\geq 2}\left(\frac{d_i}{d_j}+\frac{d_j}{d_i}\right)$$
$$= n(n-1) - 2m + \sum_{i<j:d_{i,j}\geq 2}\frac{(d_i-d_j)^2}{d_i d_j}$$
$$\geq n(n-1) - 2m + \frac{1}{\Delta^2}\left(\sum_{i<j:d_{i,j}\geq 2}(d_i^2+d_j^2) - 2\sum_{i<j:d_{i,j}\geq 2} d_i d_j\right)$$
$$= n(n-1) - 2m + \frac{1}{\Delta^2}\left(\sum_{i=1}^{n}(n-1-d_i)d_i^2 \right. \tag{10}$$
$$\left. - \sum_{i=1}^{n} d_i(2m - d_i - d_i\mu_i)\right) \text{as } d_i\mu_i = \sum_{j:j\in\Gamma(v_i)} d_j$$
$$= n(n-1) - 2m + \frac{1}{\Delta^2}\left(nM_1(G) - \sum_{i=1}^{n} d_i^3 + 2M_2(G) - 4m^2\right)$$
$$\text{as } M_1(G) = \sum_{i=1}^{n} d_i^2, \text{ and } M_2(G) = \sum_{i=1}^{n} d_i^2\mu_i. \tag{11}$$

Using (9) and (11) in (7), we get the required result (4).

Now suppose that equality holds in (4). Then $\mathbf{X} = \left(\frac{1}{\sqrt{n}}, \frac{1}{\sqrt{n}}, \ldots, \frac{1}{\sqrt{n}}\right)^T$ is an eigenvector corresponding to eigenvalue $\lambda(G)$ of $D(G)^{-1}RD(G)D(G)$. From equality in (7), we get $d \leq 2$. From equality in (8), we get $d_1 = d_2 = \cdots = d_n$. Similarly, from equality in (10), we get $d_1 = d_2 = \cdots = d_n$. Hence $G \cong K_n$ or G is isomorphic to a regular graph of diameter 2.

Conversely, one can see easily that the equality holds in (4) for complete graph K_n or for a regular graph of diameter 2. □

Remark 2.5 Our lower bound in (4) is always better than the lower bound in (1).

Zhou et al. [17] obtained the following upper bound for $\lambda(G)$ in terms of n and degree sequence $d_1, d_2, \ldots, d_n$:

Lemma 2.6 [17] *Let G be a connected graph with $n \geq 2$ vertices. Then*

$$\lambda(G) \leq \frac{1}{2}\left(n - 1 + \max_{1\leq i\leq n} d_i\right), \tag{12}$$

with equality if and only if G is a regular graph of diameter at most two.

Now we give an upper bound for $\lambda(G)$ in terms of n, m and δ only.

Theorem 2.7 *Let G be a connected graph with $n \geq 2$ vertices, m edges and minimum vertex degree δ. Then*

$$\lambda(G) \leq \frac{1}{2}\sqrt{(n-1)^2 + 3(2m-\delta)}, \tag{13}$$

with equality if and only if G is a complete graph K_n.

Proof Let $\mathbf{X} = (x_1, x_2, \cdots, x_n)^T$ be an unit eigenvector corresponding to the largest eigenvalue $\lambda(G)$ of $RD(G)$. We have

$$RD(G)\mathbf{X} = \lambda(G)\mathbf{X}. \tag{14}$$

From the i-th equation of (14) we have

$$\begin{aligned} \lambda(G)x_i &= \sum_{k:k\neq i} \frac{1}{d_{i,k}} x_k \\ &\leq \sqrt{\sum_{k:k\neq i} \frac{1}{d_{i,k}^2} \sum_{k:k\neq i} x_k^2} \text{ by Cauchy-Schwarz inequality.} \qquad (15) \end{aligned}$$

Let

$$D_i^* = \sum_{k:k\neq i}^{n} \frac{1}{d_{i,k}^2} \quad \text{i} = 1, 2, \ldots, n$$

and also let

$$D_p^* = \min_{i\in V} D_i^*.$$

Squaring both sides in (15) and taking sum for $i = 1$ to n, we get

$$\begin{aligned} \lambda^2(G) &\leq \sum_{i=1}^{n} D_i^*(1 - x_i^2) \quad \text{as } \textstyle\sum_{i=1}^n x_i^2 = 1 \text{ and } D_i^* = \displaystyle\sum_{k:k\neq i}^{n} \frac{1}{d_{i,k}^2} \qquad (16) \\ &\leq \sum_{i=1}^{n} D_i^* - D_p^* = \sum_{i=1, i\neq p}^{n} D_i^* \quad \text{as } D_p^* = \min_i\{D_i^*\}. \qquad (17) \end{aligned}$$

Since, $D_i^* = \sum_{k:k\neq i}^n \frac{1}{d_{i,k}^2} \leq d_i + \frac{1}{4}(n-1-d_i) = \frac{1}{4}(n-1+3d_i)$, that is, $\sum_{i=1,i\neq p}^n D_i^* \leq \frac{1}{4}\left((n-1)^2 + 3(2m-\delta)\right)$. Thus we have

$$\lambda^2(G) \leq \frac{1}{4}\Big((n-1)^2 + 3(2m-\delta)\Big). \tag{18}$$

Thus, we complete the first part of the proof.

Now suppose that equality holds in (13). Then all inequalities in the above argument must be equalities. From equality in (15) and (16), we get

$$d_{i,1}x_1 = d_{i,2}x_2 = \cdots = d_{i,i-1}x_{i-1} = d_{i,i+1}x_{i+1} = \cdots = d_{i,n}x_n, \quad \text{for all } i. \quad (19)$$

From equality in (16), we get

$$D_1^* = D_2^* = \cdots = D_n^* . \quad (20)$$

From equality in (18), G has diameter at most 2 and $D_i^* = \frac{1}{4}(n-1+3d_i)$, $i = 1, 2, \ldots, n$. By (20), we get $d_1 = d_2 = \cdots = d_n$, that is, G is a regular graph. If $d = 1$, then $G \cong K_n$. Otherwise, $d = 2$ and hence we have $d_{i,j} = 1$ or $d_{i,j} = 2$, for all i, j. Without loss of generality, we can assume that the shortest distance between vertex 1 and n is 2. From (19), $i = 1$ we get $x_k = 2x_n, k \in N_1$ and $x_k = x_n, k \notin N_1, k \neq 1$. Similarly, from (19), $i = n$ we get $x_k = 2x_1, k \in N_n$ and $x_k = x_1, k \notin N_n, k \neq n$. Thus we have $x_1 = x_n$ and two type of eigencomponents x_1 and $2x_1$ in eigenvector $\mathbf{X}$, which is a contradiction as G is regular graph of diameter 2. Hence G is a complete graph K_n.

Conversely, one can see easily that the equality holds in (13) for complete graph K_n. □

Remark 2.8 In order to see that the upper bound (13) is always better than the upper bound (12) for any tree except path P_n ($n \geq 5$), note that

$$\frac{1}{2}(n-1+\Delta) \geq \frac{1}{2}\sqrt{(n-1)^2 + 3(2m-\delta)}.$$

holds if and only if

$$\Delta^2 + 2\Delta(n-1) \geq 3(2m-\delta)$$

which is equivalent to

$$2n(\Delta-3) + (\Delta-1)^2 + 8 \geq 0,$$

which, evidently, is always obeyed. Similarly, one can easily check that the upper bound (13) is always better than the upper bound (12) for graphs of maximum degree $\Delta = n-1$.

Remark 2.9 The lower and upper bounds given by (4) and (13), respectively, are equal when G is a complete graph K_n.

3 The Nordhaus-Gaddum-type result for the maximum eigenvalue of the reciprocal distance matrix

Zhou et al. [17] obtained the following Nordhaus-Gaddum-type result for the maximum eigenvalue of the reciprocal distance matrix in terms of n only:

Lemma 3.1 *Let G be a connected graph on $n \geq 4$ vertices with a connected $\overline{G}$. Then*

$$n < \lambda(G) + \lambda(\bar{G}) < 2n - 3. \tag{21}$$

Now we give the lower bound for $\lambda(G) + \lambda(\overline{G})$:

Theorem 3.2 *Let G be a connected graph on $n \geq 4$ vertices with a connected $\bar{G}$. Then*

$$\lambda(G) + \lambda(\overline{G}) \geq (n-1)\left(1 + \frac{1}{k}\right) \tag{22}$$

where $k = \max\{d, \overline{d}\}$ and d, $\overline{d}$ are the diameter of G and $\overline{G}$, respectively. Moreover, the equality holds in (22) if and only if both G and $\overline{G}$ are regular graph of diameter 2.

Proof Using the inequality (1) from Lemma 2.1 we arrive at

$$\lambda(G) + \lambda(\overline{G}) \geq \frac{2m + 2\overline{m}}{n} + \frac{n(n-1) - 2m}{nd} + \frac{n(n-1) - 2\overline{m}}{n\overline{d}} \tag{23}$$

where $\overline{m}$ and $\overline{d}$ are, respectively, the number of edges and diameter of $\overline{G}$. Since $m + \overline{m} = \frac{n(n-1)}{2}$ and $k = \max\{d, \overline{d}\}$, we get (22) from (23). First part of the proof is over.

Now suppose that equality holds in (22). Then the equality holds in (23) and $k = d = \overline{d}$. From equality in (23), we get both G and $\overline{G}$ are regular graph of diameter 2, by Lemma 2.1. Hence both G and $\overline{G}$ are regular graph of diameter 2.

Conversely, let both G and $\overline{G}$ be regular graph of diameter 2. Then $\lambda(G) = \frac{n+r-1}{2}$ and $\lambda_1(\overline{G}) = \frac{2(n-1)-r}{2}$. Hence $\lambda(G) + \lambda_1(\overline{G}) = \frac{3}{2}(n-1)$. □

Example 3.3 For $G = C_5$ (C_5 is a cycle of length 5), we have $\lambda(C_5) + \lambda(\overline{C}_5) = 6$, since complement of C_5 is also C_5.

Remark 3.4 It is easily see that our lower bound (22) is always better than (21) as $2 \leq k \leq n - 1$.

Here we give the upper bound for $\lambda(G) + \lambda(\overline{G})$ in terms of n, Δ and δ.

Theorem 3.5 *Let G be a connected graph on $n \geq 4$ vertices with a connected $\overline{G}$. Then*

$$\lambda(G) + \lambda(\overline{G}) \leq \sqrt{\frac{1}{2}[5(n-1)^2 + 3(\Delta - \delta)]}. \tag{24}$$

Proof Using the inequality (13) from Theorem 2.7 we arrive at

$$\begin{aligned} \lambda(G) + \lambda(\overline{G}) &\leq \frac{1}{2}\sqrt{(n-1)^2 + 3(2m - \delta)} + \frac{1}{2}\sqrt{(n-1)^2 + 3(2\overline{m} - \overline{\delta})}\,. \\ &= \frac{1}{2}\sqrt{(n-1)^2 + 3(2m - \delta)} + \frac{1}{2}\sqrt{4(n-1)^2 - 6m + 3\Delta} \quad (25) \\ &\text{as } 2\overline{m} = n(n-1) - 2m \text{ and } \Delta = n - 1 - \overline{\delta}, \end{aligned}$$

where $\overline{m}$ and $\overline{\delta}$ are, respectively, the number of edges and the minimum vertex degree of $\overline{G}$. Now we consider a function

$$f(m) = \sqrt{(n-1)^2 + 3(2m-\delta)} + \sqrt{4(n-1)^2 - 6m + 3\Delta}.$$

It is easy to show that

$$f(m) \leq f\left(\frac{(n-1)^2 + \Delta + \delta}{4}\right) = 2\sqrt{\frac{1}{2}[5(n-1)^2 + 3(\Delta - \delta)]}. \tag{26}$$

From (25) and (26), we get the required result (24). □

Remark 3.6 In order to see that the upper bound (24) is always better than the upper bound (21) for any graphs, note that

$$(2n-3)^2 \geq \frac{1}{2}\left[5(n-1)^2 + 3(\Delta - \delta)\right]$$

holds if and only if

$$\left(n - \frac{1}{3}\right)^2 + \frac{38}{9} - (\Delta - \delta) \geq 0$$

which, evidently, is always obeyed.

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