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On Harary Matrix, Harary Index and Harary Energy

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Abstract

Recently, a new molecular graph matrix, Harary matrix, was defined in honor of Professor Frank Harary, and new graph invariants (local and global) based on it were also defined and researched, Harary index is one of these invariants. The Harary matrix can be used to derive a variant of the Balaban index, Harary index was also successfully tested in several structure-property relationships, so it is very meaningful to research their mathematical properties and chemical applications. As a class of graph energy, Harary energy was introduced not long ago. In this paper, we obtain some results about eigenvalues of Harary matrix, then by these results, we get some bounds of Harary index. Moreover, we obtain some bounds of Harary energy.

1. Introduction

As we know, in many instances the distant atoms influence each other much less than near atoms. To research this interaction, Ivanciuc et al. [1] define a new molecular graph matrix, Harary matrix (called it initially the reciprocal distance matrix [2]), which was successfully used in a study concerning computer generation of acyclic graphs based on local vertex invariants and topological indices [3]. The Harary index is derived from the Harary matrix and has a number of interesting properties, it has shown a modest success in structure-property correlations [4-8],

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but its use in combination with other molecular descriptors appears to be very efficacious in improving the QSPR (quantitative structure-property relationship) models [9]. Recently there has been a tremendous research activity in graph energy, as a class of graph energy, Harary energy will inevitably arouse the interest of chemists.

Let $G = (V, E)$ be a 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 $d_{i,j}$ be the distance between the vertices v_i and v_j in G. The Harary matrix $RD(G)$ of G is an $n \times n$ matrix $(RD_{i,j})$ such that [10, 11]

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

The Harary index of the graph G, denoted by $H(G)$, defined as

$$H(G) = \frac{1}{2} \sum_{i=1}^{n} \sum_{j=1}^{n} RD_{i,j} = \sum_{i<j} RD_{i,j} .$$

Let $\mu_1, \mu_2, \ldots, \mu_n$ $(\mu_1 \geq \mu_2 \geq \cdots \geq \mu_n)$ be the eigenvalues of RD. The Harary energy of the graph G, denoted by $HE(G)$, defined as

$$HE(G) = \sum_{i=1}^{n} | \mu_i | .$$

Since RD be a real symmetric matrix, its eigenvalues are all real. Ivanciuc et al. [12] proposes to use the maximum eigenvalues of distance-based matrices as structural descriptors. The lower and upper bounds of the maximum eigenvalues of Harary matrix, and the Nordhaus-Gaddum-type results for it were obtained in [13, 14]. Mathematical properties and applications of Harary index are reported in [15-21]. Some lower and upper bounds for Harary energy of connected (n, m)-graphs were obtain in [22].

This paper is organized as follows. In the Section 2, we get the Harary matrix spectrum of some graphs of diameter 2 and 3. In the Section 3, the upper bounds for the maximum RD-eigenvalues of bipartite graph are obtained. In the Section 4, the upper bounds for the Harary index of bipartite graph are obtained. In the Section 5, the upper bounds for the Harary energy of some graphs are obtained.

All graphs considered in this paper are simple. our spectral graph theoretic terminology follows that of the book [23, 24].

2. Harary matrix spectrum of graphs of diameter 2 or 3

Moore and Moser showed [25] that almost all graphs are of diameter two. Thus a discussion of graphs of small diameter pertains to almost all graphs.

Let G be a graph of, its adjacency matrix is A, and the adjacency matrix of its complement $\overline{G}$ is $\overline{A}$, then $d(u,v) = 1$ if u adj v in G, and $d(u,v) = 2$ if u adj v in $\overline{G}$. Thus the Harary matrix of G is $A + \frac{1}{2}\overline{A}$.

Theorem 1. Let G be an r-regular graph of diameter 2, its adjacency spectrum be $spec(G) = \{r, \lambda_2, \ldots, \lambda_n\}$. Then the RD-spectrum of G is

$$spec_{RD}(G) = \left\{\frac{1}{2}(n+r-1), \frac{1}{2}(\mu_2 - 1), \ldots, \frac{1}{2}(\mu_n - 1)\right\} .$$

Proof. Because the Harary matrix of G is $A + \frac{1}{2}\overline{A}$ and $\overline{A} = J - I - A$, where J denote the all-1 matrix and I denote the unit matrix, so $RD(G) = \frac{1}{2}(J - I + A)$. Note that eigenvectors of A are also eigenvectors of J and $spec(J) = \{n, 0, \ldots, 0\}$, we can get the result. □

Before proving the theorem 2, we need follow lemma.

Lemma 1.[26] Let

$$\begin{pmatrix} A_0 & A_1 \\ A_1 & A_0 \end{pmatrix}$$

be a symmetric 2×2 block matrix. Then the spectrum of A is the union of the spectra of $A_0 + A_1$ and $A_0 - A_1$.

Theorem 2. Let G be an r-regular graph of diameter 1 or 2 with an adjacency matrix A and $spec(G) = \{r, \lambda_2, \ldots, \lambda_n\}$. Then $H = G \times K_2$ is $(r+1)$-regular and of diameter 2 or 3 with

$$spec_{RD}(H) = \begin{pmatrix} \frac{5}{6}n + \frac{2}{3}r + \frac{1}{6} & \frac{2}{3}\lambda_i + \frac{1}{6} & \frac{1}{6}n + \frac{1}{3}r - \frac{7}{6} & \frac{1}{3}\lambda_i - \frac{7}{6} \\ 1 & 1 & 1 & 1 \end{pmatrix} , \; i = 2, \ldots, n .$$

Proof. Since G is of diameter 1 or 2, its Harary matrix is $A + \frac{1}{2}\overline{A}$. Then the Harary matric of H is of the form

$$\begin{pmatrix} A + \frac{1}{2}\overline{A} & J - \frac{1}{2}A - \frac{2}{3}\overline{A} \\ J - \frac{1}{2}A - \frac{2}{3}\overline{A} & A + \frac{1}{2}\overline{A} \end{pmatrix}.$$

By lemma 1, the spectrum of RD is the union of the spectra of

$$A + \tfrac{1}{2}\overline{A} + J - \tfrac{1}{2}A - \tfrac{2}{3}\overline{A} = J + \tfrac{1}{2}A - \tfrac{1}{6}\overline{A} = \tfrac{5}{6}J + \tfrac{1}{6}I + \tfrac{2}{3}A$$

and

$$A + \tfrac{1}{2}\overline{A} - J + \tfrac{1}{2}A + \tfrac{2}{3}\overline{A} = \tfrac{3}{2}A + \tfrac{7}{6}\overline{A} - J = \tfrac{1}{3}A + \tfrac{1}{6}J - \tfrac{7}{6}I.$$

From this we get the required result. □

3. Spectral radius of Harary matrix of bipartite graph

Theorem 3. Let G be a connected bipartite (n,m)-graph with bipartite $V(G) = A \bigcup B$, $|A| = p$, $|B| = q$. Then

$$\mu_1(G) \le \frac{1}{4}(n - 2 + \sqrt{n^2 + 12pq}) \tag{1}$$

with equality if and only if G is a complete bipartite graph $K_{p,q}$.

Proof. Since G is bipartite graph, we can assume that $A = \{1, 2, \ldots, p\}$, and $B = \{p+1, p+2, \ldots, p+q\}$, where $p + q = n$. Let $X = (x_1, x_2, \ldots, x_n)^T$ be an eigenvector of $RD(G)$ corresponding to the maximum eigenvalue $\mu_1(G)$. Then we have $RD(G)X = \mu_1(G)X$. We can assume that $x_i = max_{k\in A} x_k$, and $x_j = max_{k\in B} x_k$.

For $i \in A$,

$$\mu_1(G)x_i = \sum_{k=1,k\neq i}^{p} \frac{1}{d_{i,k}} \cdot x_k + \sum_{k=p+1}^{p+q} \frac{1}{d_{i,k}} \cdot x_k \le \frac{1}{2}(p-1)x_i + qx_j \,. \tag{2}$$

For $i \in B$,

$$\mu_1(G)x_i = \sum_{k=1}^{p} \frac{1}{d_{j,k}} \cdot x_k + \sum_{k=p+1,k\neq j}^{p+q} \frac{1}{d_{j,k}} \cdot x_k \le px_i + \frac{1}{2}(q-1)x_j \,. \tag{3}$$

Since G is a connected graph, $x_k > 0$ for all $k \in V$. From (2) and (3), we can get $[\mu_1 - \frac{1}{2}(p-1)][\mu_1 - \frac{1}{2}(q-1)] \le pq$ as $x_i,\ x_j > 0$, that is

$$\mu_1^2 - \frac{1}{2}(p+q-2)\mu_1 + \frac{1}{4}(1-p-q-3pq) \le 0 \,.$$

From this we get the required result (1).

Now suppose that equality holds in (1). Then all inequalities in the above argument must be equalities. From equality in (2), we get

$$x_k = x_j \text{ and } ik \in E(G) \text{ for all } k \in B \,.$$

From equality in (3), we get

$$x_k = x_i \text{ and } jk \in E(G) \text{ for all } k \in A \,.$$

Thus each vertex in each set is adjacent to all the vertices on the other set and vice versa. Hence G is a complete bipartite graph $K_{p,q}$.

Conversely, one can easily to see that (1) hold for $K_{p,q}$. □

Theorem 4. Let G be a connected bipartite (n, m)-graph with bipartite $V(G) = A \bigcup B$, $|A| = p$, $|B| = q$, $p + q = n$. Let $\triangle_A$ and $\triangle_B$ be maximum degrees among vertices from A and B, respectively. Then

$$\mu_1(G) \leq \frac{1}{4}(n-2) + \frac{1}{12}\sqrt{25 + 9n^2 + 8p\triangle_A + 8q\triangle_B + 16\triangle_A\triangle_B - 25n - 5pq}$$

with equality if and only if G is a complete bipartite graph $K_{p,q}$ or G is a semi-regular graph with every vertex eccentricity equal 3.

Proof. Let $A = \{1, 2, \ldots, p\}$, $B = \{p+1, p+2, \ldots, p+1\}$. Let $X = (x_1, x_2, \ldots, x_n)^T$ be a Perron eigenvector of $RD(G)$ corresponding to the maximum eigenvalue $\mu_1(G)$, such that

$$x_i = max_{k \in A} x_k \text{ and } x_j = max_{k \in B} x_k \ .$$

From the eigenvalue equation $RD(G)X = \mu_1(G)X$, written for the component x_i we have

$$\begin{aligned} \mu_1(G)x_i &= \sum_{k=1, k\neq i}^{p} \frac{1}{d_{i,k}} \cdot x_k + \sum_{k=p+1}^{p+q} \frac{1}{d_{i,k}} \cdot x_k \\ &\leq \tfrac{1}{2}(p-1)x_i + d_i x_j + \tfrac{1}{3}(q - d_i)x_j \\ &\leq \tfrac{1}{2}(p-1)x_i + \tfrac{1}{3}(q + 2\triangle_A)x_j \ . \end{aligned}$$

Analogously for the component x_j we have

$$\begin{aligned} \mu_1(G)x_j &= \sum_{k=1}^{p} \frac{1}{d_{j,k}} \cdot x_k + \sum_{k=p+1, k\neq i}^{p+q} \frac{1}{d_{j,k}} \cdot x_k \\ &\leq d_j x_i + \tfrac{1}{3}(p - d_j)x_i + \tfrac{1}{2}(q-1)x_j \\ &\leq \tfrac{1}{2}(q-1)x_j + \tfrac{1}{3}(p + 2\triangle_B)x_i \ . \end{aligned}$$

Combining these two inequalities, it follows

$$[\mu_1 - \tfrac{1}{2}(p-1)][\mu_1 - \tfrac{1}{2}(q-1)] \leq \tfrac{1}{9}(q + 2\triangle_A)(p + 2\triangle_B),$$

Since $x_k > 0$ for $1 \leq k \leq p + q$,

$$\mu_1^2 - \tfrac{1}{2}(p+q-2)\mu_1 + \tfrac{1}{36}(9 + 5pq - 9p - 9q - 8p\triangle_A - 8q\triangle_B - 16\triangle_A\triangle_B) \leq 0.$$

From this inequality, we get the result.

For the case of equality, we have $x_i = x_k$ for $k = 1, 2, \ldots, p$ and $x_j = x_k$ for $k = p+1, p+2, \ldots, p+q$. This means that eigenvector x has at most two different coordinates, the degrees of vertices in A are equal to $\triangle_A$, and the degrees of vertices in B are equal to $\triangle_B$, implying that G is a semi-regular graph. If G is not a complete bipartite graph, it follows from $p\triangle_A = q\triangle_B$ that $\triangle_A < q$ and $\triangle_B < p$ and the eccentricity of every vertex must be equal to 3. □

4. Bounds for Harary index of bipartite graph

Recently, the research is intense about bounds of Harary index. The general and Nordhaus-Gaddum-type bounds for it were obtained in [19], and results of trees also have been given in [27], here we give bounds for Harary index of bipartite graph.

Lemma 2. (Rayleigh-Ritz) [28] If A is a symmetric $n \times n$ matrix with eigenvalues $\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_n$, then for any $X \in R^n (X \neq 0)$,

$$X^T A X \leq \lambda_1 X^T X.$$

Equality holds if and only if X is an eigenvector of A corresponding to the largest eigenvalue λ_1.

Theorem 5. Let G be a connected bipartite (n, m)-graph with bipartite $V(G) = A \bigcup B$, $|A| = p$, $|B| = q$. Then

$$H(G) \leq \frac{1}{8} n(n - 2 + \sqrt{n^2 + 12pq})$$

with equality if and only if G is a complete bipartite graph $K_{p,q}$.

Proof. Because $RD(G)$ be a real symmetric matrix, if we choose $X = (1, 1, \ldots, 1)$ and $A = RD(G)$ in the lemma 2, and combine theorem 3, we can get

$$H(G) \leq \frac{n}{2}\mu(G) \leq \frac{1}{8} n(n - 2 + \sqrt{n^2 + 12pq})$$

□

Analogously, combining theorem 4 and lemma 2, we can get follow theorem.

Theorem 6. Let G be a connected bipartite (n, m)-graph with bipartite $V(G) = A \bigcup B$, $|A| = p$, $|B| = q$, $p + q = n$. Let $\triangle_A$ and $\triangle_B$ be maximum degrees among vertices from A and B, respectively. Then

$$H(G) \leq \frac{n}{8}(n - 2) + \frac{n}{24}\sqrt{25 + 9n^2 + 8p\triangle_A + 8q\triangle_B + 16\triangle_A\triangle_B - 25n - 5pq}$$

with equality if and only if G is a complete bipartite graph $K_{p,q}$ or G is a semi-regular graph with every vertex eccentricity equal 3.

5. Bounds for Harary energy

Lemma 3.[22] Let G be a connected (n, m)-graph and $\mu_1, \mu_2, \ldots, \mu_n$ $(\mu_1 \geq \mu_2 \geq \cdots \geq \mu_n)$ be the eigenvalues of RD. Then

$$\sum_{i=1}^{n} \mu_i = 0$$

and

$$\sum_{i=1}^{n} \mu_i^2 = 2 \sum_{1 \le i < j \le n} \left(\frac{1}{d_{ij}} \right)^2 .$$

Lemma 4.[14] Let G be a connected graph with $n \geq 2$ vertices, m edges and minimum vertex degree δ. Then

$$\mu_1 \le \frac{1}{2} \sqrt{n - 1 + 3(2m - \delta)}$$

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

Theorem 7. Let G be a connected graph with $n \geq 2$ vertices. m edges and minimum vertex degree δ. Then

$$HE(G) \le \frac{1}{2} \sqrt{n - 1 + 3(2m - \delta)} + \sqrt{(n-1)\left(2 \sum_{1 \le i < j \le n} \left(\frac{1}{d_{ij}} \right)^2 - \frac{1}{4}(n-1)^2 - 3(2m - \delta) \right)}$$

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

Proof. By the define of Harary energy, combining Cauchy-Schwartz inequality and lemma 3, we can get

$$\begin{aligned} (HE(G) - \mu_1)^2 &= \left(\sum_{i=2}^{n} | \mu_i | \right)^2 \\ &\le (n-1) \left(\sum_{i=1}^{n} \mu_i^2 - \mu_1^2 \right) \\ &= (n-1) \left(2 \sum_{1 \le i < j \le n} \left(\frac{1}{d_{ij}} \right)^2 - \mu_1^2 \right) \end{aligned}$$

then

$$HE(G) \le \mu_1 + \sqrt{(n-1)\left(2 \sum_{1 \le i < j \le n} \left(\frac{1}{d_{ij}} \right)^2 - \mu_1^2 \right)} \tag{4}$$

By lemma 4, the theorem follows.

Note that equality holds in lemma 4, one can easily to see that with equality if and only if G is a complete graph K_n. □

Remark: In [28], authors give the upper of $HE(G)$ which is $\sqrt{2n \sum_{1 \le i < j \le n} \left(\frac{1}{d_{ij}} \right)^2}$, after simple comparison, the reader can know our result is better than that.

Analogously, combining theorem 3 and the inequality (4) in theorem 7, we can obtain follow theorem.

Theorem 8. Let G be a connected bipartite (n, m)-graph with bipartite $V(G) = A \bigcup B$, $|A| = p$, $|B| = q$. Then

$$HE(G) \leq \frac{1}{4}\left(n - 2 + \sqrt{n^2 + 12pq}\right) + \sqrt{(n-1)\left(2\sum_{1 \leq i < j \leq n}\left(\frac{1}{d_{ij}}\right)^2 - \frac{1}{16}\left(n - 2 + \sqrt{n^2 + 12pq}\right)^2\right)}$$

References

[1] O. Ivanciuc, T. S. Balaban, A. T. Balaban, Design of topological indices. Part 4. Reciprocal distance matrix, related local vertex invariants and topological indices, *J. Math. Chem.* **12** (1993) 309–318.

[2] D. Janežič, A. Miličević, S. Nikolić, N. Trinajstić, *Graph Theoretical Matrices in Chemistry*, Univ. Kragujevac, Kragujevac, 2007.

[3] T. S. Balaban, P. A. Filip, O. Ivanciuc. Computer generation of acyclic graphs based on local vertex invariants and topological indices. Derived canonical labelling and coding of trees and alkanes, *J. Math. Chem.* **11** (1992) 79–105.

[4] B. Lučić, A. Miličević, S. Nikolić, N. Trinajstić, Harary index – Twelve years later, *Croat. Chem. Acta* **75** (2002) 847–868.

[5] J. Devillers, A. T. Balaban (Eds.), *Topological Indices and Related Descriptors in QSAR and QSPR*, Gordon and Breach, Amsterdam, 1999.

[6] R. Todeschini, V. Consonni, *Handbook of Molecular Descriptors*, Weinheim, Wiley–VCH, 2000.

[7] Z. Mihalić, N. Trinajstić, A graph–theoretical approach to structure–property relationships, *J. Chem. Educ.* **69** (1999) 701–712.

[8] O. Ivanciuc, QSAR comparative study of Wiener descriptors for weighted molecular graphs, *J. Chem. Inf. Comput. Sci.* **40** (2000) 1412–1422.

[9] N. Trinajstić, S. Nikolić, S. C. Basak, I. Lukovits, Distance indices and their hyper–counterparts: Intercorrelation and use in the structure–property modeling, *SAR QSAR Environ. Res.* **12** (2001) 31–54.

[10] D. Plavšić, S. Nikolić, N. Trinajstić, Z. Mihalić, On the Harary index for the characterization of chemical graphs, *J. Math. Chem.* **12** (1993) 235–250.

[11] O. Ivanciuc, T. S. Balaban, A. T. Balaban, Chemical graphs with degenerate topological indices based on information on distances, *J. Math. Chem.* **12** (1993) 21–33.

[12] O. Ivanciuc, T. Ivanciuc, A. T. Balaban, Quantitative structure–property relationship evaluation of structural descriptors derived from the distance and reverse Wiener matrices, *Internet El. J. Mol. Des.* **1** (2002) 467–487.

[13] B. Zhou, N. Trinajstić, Maximum eigenvalues of the reciprocal distance matrix and the reverse Wiener matrix, *Int. J. Quantum Chem.* **108** (2008) 858–864.

[14] K. C. Das, Maximum eigenvalues of the reciprocal distance matrix, *J. Math. Chem.* **47** (2010) 21–28.

[15] K. C. Das, B. Zhou, N. Trinajstić, Bounds on Harary index, *J. Math. Chem.* **46** (2009) 1369–1376.

[16] E. Estrada, L. Rodríguez, Matrix algebraic manipulation of molecular graphs. 2. Harary and MTI–like molecular descriptors, *MATCH Commun. Math. Comput. Chem.* **35** (1997) 157–167.

[17] L. Feng, A. Ilić, Zagreb, Harary and hyper–Wiener indices of graphs with a given matching number, *Appl. Math. Lett.* **23** (2010) 943–948.

[18] K. Xu, N. Trinajstić, Hyper-Wiener and Harary indices of graphs with cut edges, *Util. Math.* **84** (2011) 153–163.

[19] B. Zhou, X. Cai, N. Trinajstić, On the Harary index, *J. Math. Chem.* **44** (2008) 611–618.

[20] K. Xu, K. C. Das, On Harary index of graphs, *Discr. Appl. Math.* **159** (2011) 1631–1640.

[21] B. Zhou, Z. Du, N. Trinajstić, Harary index of landscape graphs, *Int. J. Chem. Model.* **1** (2008) 35–44.

[22] A. D. Gungor, A. S Çevik, On the Harary energy and Harary Estrada index of a graph, *MATCH Commun. Math. Comput. Chem.* **64** (2010) 280–296.

[23] D. M. Cvetković, M. Doob, H. Sachs, *Spectra of Graphs – Theory and Application*, Academic Press, New York, 1980.

[24] A. E. Brouwer, W. H. Haemers, *Spectra of Graphs*, Springer, Berlin, 2012.

[25] F. Buckley, F. Harary, *Distance in Graphs*, Addison–Wesley, Redwood, 1990.

[26] P. J. Davis, *Circulant Matrices*, Wiley, New York, 1979.

[27] A. Ilić, G. Yu, L. Feng, The Harary index of trees, arXiv:1104.0920v3 [math.CO], (2011).

[28] F. Zhang, *Matrix Theory Basic Results and Techniques*, Springer–Verlag, New York, 1999.