Applied Mathematics and Computation 266 (2015) 937–945

Contents lists available at ScienceDirect

Applied Mathematics and Computation

journal homepage: www.elsevier.com/locate/amc

On graphs with maximum Harary spectral radius☆

Fei Huang, Xueliang Li*, Shujing Wang

Center for Combinatorics and LPMC-TJKLC, Nankai University, Tianjin 300071, China

ARTICLE INFO

MSC:
05C50
15A18
92E10

Keywords:
Harary matrix
Harary spectral radius
Matching number
Cut edge

ABSTRACT

Let G be a connected (molecular) graph with vertex set $V(G)=\{v_1, v_2, \ldots, v_n\}$. The Harary matrix $RD(G)$ of G, which is also known as the reciprocal distance matrix, is an $n \times n$ matrix whose (i, j)-entry is equal to $\frac{1}{d_{ij}}$ if $i \neq j$ and 0 otherwise, where d_{ij} is the distance of v_i and v_j in G. The spectral radius $\rho(G)$ of the Harary matrix $RD(G)$ has been proposed as a structure-descriptor. In this paper, we characterize graphs with maximum spectral radius of the Harary matrix in three classes of simple connected graphs with n vertices: graphs with fixed matching number, bipartite graphs with fixed matching number, and graphs with given number of cut edges, respectively.

1. Introduction

The physical, chemical, and biological properties of chemical compounds are ultimately determined by the molecular structure. An efficient way of coding the topology of a molecular structure is represented by topological indices (or structural descriptors), where a topological index is a numerical representation of the molecular structure derived from the corresponding molecular graph. Since the distance matrix and related matrices, based on graph–theoretical distances [12], are rich sources of many graph invariants (topological indices) that have found use in structure–property–activity modeling [5,8,15,16,17], it is of interest to study spectra and polynomials of these matrices [1,9]. As we know, in many instances the distant atoms influence each other much less than near atoms. The Harary matrix $RD(G)$ of G, which is also known as the reciprocal distance matrix was introduced by Ivanciuc et al. [10] as an important molecular matrix to research this interaction.

We consider simple (molecular) graphs, that is, graphs without multiple edges and loops. Undefined notation and terminology can be found in [2]. Let G be a simple graph with vertex set $V(G)=\{v_1, v_2, \ldots, v_n\}$ and edge set $E(G)$. Let $N_G(v)$ be the neighborhood of the vertex v of G, and d_{ij} be the distance (i.e., the number of edges of a shortest path) between the vertices v_i and v_j in G.

We restate the definition of the Harary matrix here. The Harary matrix $RD(G)$ of G is an $n \times n$ matrix (RD_{ij}) such that

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

Since RD is a real symmetric matrix, its eigenvalues are all real. Let $\rho(G)$ be the spectral radius(the largest eigenvalue) of $RD(G)$, called the Harary spectral radius. Ivanciuc et al. [11] proposes to use the maximum eigenvalues of distance-based matrices as structural descriptors. It is shown in [11] that the Harary spectral radius is able to produce fair quantitative structure–property

☆ This work was supported by NSFC no.11371205 and PCSIRT.

* Corresponding author. Tel.: +86 2223506800.
E-mail addresses: huangfei06@126.com (F. Huang), lxl@nankai.edu.cn (X. Li), wang06021@126.com (S. Wang).

http://dx.doi.org/10.1016/j.amc.2015.05.146

relationships (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 have recently attracted attention of mathematical chemists.

The lower and upper bounds of the maximum eigenvalues of the Harary matrix, and the Nordhaus–Gaddum-type results for it were obtained in [4,18]. Cui and Liu [3] proposed some more results about eigenvalues of Harary matrices; also, they got some bounds of the Harary index and Harary energy by these results. Some lower and upper bounds for the Harary energy of connected (n, m)-graphs were obtained in [7].

A matching in a graph is a set of pairwise nonadjacent edges. A maximum matching is one which covers as many vertices as possible. The number of edges in a maximum matching of a graph G is called the matching number of G and is denoted by $\alpha'(G)$. In this paper we characterize graphs with maximum spectral radius of the Harary matrix in three classes of simple connected graphs with n vertices: graphs with fixed matching number, bipartite graphs with fixed matching number, and graphs with given number of cut edges, respectively.

2. Preliminaries

By the Perron–Frobenius theorem, the Harary spectral radius of a connected graph G corresponds to a unique positive unit eigenvector $X = (x_1, x_2, \ldots, x_n)^T$, called principal eigenvector of $RD(G)$. Then

$$\rho(G)x_i = \sum_{j\neq i} \frac{1}{d_{ij}} x_j. \tag{1}$$

The following lemma is an immediate consequence of Perron–Frobenius theorem.

Lemma 2.1. *Let G be a connected graph with $u, v \in V(G)$ and $uv \notin E(G)$. Then $\rho(G) < \rho(G + uv)$.*

Let G be a connected graph, and H a subgraph of G. We know that H can be obtained from G by deleting edges, and possibly vertices.

Corollary 2.2. *If H is a proper subgraph of a connected graph G, then $\rho(H) < \rho(G)$.*

Lemma 2.3. *Let G be a connected graph with $v_r, v_s \in V(G)$. If $N_G(v_r) \setminus \{v_s\} = N_G(v_s) \setminus \{v_r\}$, then $x_r = x_s$.*

Proof. From Eq. (1), we know that

$$\rho(G)x_r = \sum_{j\neq r} \frac{1}{d_{rj}} x_j = \frac{1}{d_{rs}} x_s + \sum_{j\neq s,r} \frac{1}{d_{rj}} x_j$$

and

$$\rho(G)x_s = \sum_{j\neq s} \frac{1}{d_{sj}} x_j = \frac{1}{d_{sr}} x_r + \sum_{j\neq s,r} \frac{1}{d_{sj}} x_j.$$

Since $N_G(v_r) \setminus \{v_s\} = N_G(v_s) \setminus \{v_r\}$, we have that $d_{rj} = d_{sj}$ for $j \neq s, r$. Then

$$\rho(G)(x_r - x_s) = -\frac{1}{d_{sr}}(x_r - x_s),$$

and thus $x_r = x_s$. $\square$

3. Graphs with given matching number

The methods used in this section are a little similar to those for the distance matrix [14]. However, we find out some errors in the proof of the results for the distance matrix. We modify their techniques here and provide a correct proof for our result.

Let $G_1 \cup \cdots \cup G_k$ be the vertex–disjoint union of the graphs $G_1, \ldots, G_k$ $(k \geq 2)$, and $G_1 \vee G_2$ be the graph obtained from $G_1 \cup G_2$ by joining each vertex of G_1 to each vertex of G_2.

Lemma 3.1. *Let $G_1 = K_s \vee (K_{n_1} \cup K_{n_2} \cup \cdots \cup K_{n_k})$ and $G_2 = K_s \vee (K_{n_1-1} \cup K_{n_2+1} \cup \cdots \cup K_{n_k})$. If $n_2 \geq n_1 \geq 2$, then $\rho(G_1) < \rho(G_2)$.*

Proof. Let $\rho(G_1)$ be the Harary spectral radius of G_1 and X the corresponding principal eigenvector. By Lemma 2.3, X can be written as

$$X = (\underbrace{y_1, \ldots y_1}_{n_1}, \underbrace{y_2, \ldots y_2}_{n_2}, \ldots, \underbrace{y_k, \ldots y_k}_{n_k}, \underbrace{y_0, \ldots y_0}_{s}).$$

From Eq. (1), we have

$$\rho(G_1)y_1 = (n_1 - 1)y_1 + \frac{1}{2}n_2 y_2 + \sum_{i=3}^{k} \frac{1}{2} n_i y_i + s y_0,$$

$$\rho(G_1)y_2 = \frac{1}{2}n_1y_1 + (n_2-1)y_2 + \sum_{i=3}^{k}\frac{1}{2}n_iy_i + sy_0.$$

It implies that

$$\rho(G_1)(y_1-y_2) = \frac{1}{2}n_1y_1 - y_1 - \frac{1}{2}n_2y_2 + y_2,$$

that is,

$$\Big(\rho(G_1)+1-\frac{1}{2}n_1\Big)y_1 = \Big(\rho(G_1)+1-\frac{1}{2}n_2\Big)y_2.$$

Note that K_{s+n_2} is a subgraph of G_1 and $n_2 \geq n_1$. By Corollary 2.2 we have that

$$\rho(G_1) > \rho(K_{s+n_2}) = s+n_2-1 \geq n_2.$$

Then we have that

$$y_1 \leq y_2.$$

From the definition of the Harary matrix, we know that

$$RD(G_1) = \begin{pmatrix} (J-I)_{n_1\times n_1} & \frac{1}{2}J_{n_1\times n_2} & \cdots & \frac{1}{2}J_{n_1\times n_k} & J_{n_1\times s} \\ \frac{1}{2}J_{n_2\times n_1} & (J-I)_{n_2\times n_2} & \cdots & \frac{1}{2}J_{n_2\times n_k} & J_{n_2\times s} \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ \frac{1}{2}J_{n_k\times n_1} & J_{n_k\times n_2} & \cdots & (J-I)_{n_k\times n_k} & J_{n_k\times s} \\ J_{s\times n_1} & J_{s\times n_2} & \cdots & J_{s\times n_k} & (J-I)_{s\times s} \end{pmatrix}$$

and

$$RD(G_2) = \begin{pmatrix} (J-I)_{(n_1-1)\times(n_1-1)} & \frac{1}{2}J_{(n_1-1)\times(n_2+1)} & \cdots & \frac{1}{2}J_{(n_1-1)\times n_k} & J_{(n_1-1)\times s} \\ \frac{1}{2}J_{(n_2+1)\times(n_1-1)} & (J-I)_{(n_2+1)\times(n_2+1)} & \cdots & \frac{1}{2}J_{(n_2+1)\times n_k} & J_{n_2\times s} \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ \frac{1}{2}J_{n_k\times(n_1-1)} & J_{n_k\times(n_2+1)} & \cdots & (J-I)_{n_k\times n_k} & J_{n_k\times s} \\ J_{s\times(n_1-1)} & J_{s\times(n_2+1)} & \cdots & J_{s\times n_k} & (J-I)_{s\times s} \end{pmatrix}.$$

Thus

$$RD(G_2)-RD(G_1) = \begin{pmatrix} 0_{(n_1-1)\times(n_1-1)} & -\frac{1}{2}J_{(n_1-1)\times 1} & 0_{(n_1-1)\times n_2} & 0 \\ -\frac{1}{2}J_{1\times(n_1-1)} & 0_{1\times 1} & \frac{1}{2}J_{1\times n_2} & 0 \\ 0_{n_2\times(n_1-1)} & \frac{1}{2}J_{n_2\times 1} & 0_{n_2\times n_2} & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}.$$

Hence

$$\begin{aligned} \rho(G_2)-\rho(G_1) &\geq X^TRD(G_2)X - X^TRD(G_1))X \\ &= X^T(RD(G_2)-RD(G_1))X = n_2y_1y_2 - (n_1-1)y_1^2 \\ &> 0. \end{aligned}$$

We complete the proof. □

We will consider graphs with form $G = K_s \vee (\overline{K_{k-1}} \cup K_{2t+1})$ and characterize extremal graphs in terms of the relation between t and k.

Lemma 3.2. *Let $G = K_s \vee (\overline{K_{k-1}} \cup K_{2t+1})$ with $t \geq 1$, $k \geq 3$, and $G' = K_{s+t} \vee \overline{K_{k+t}}$. If $t \leq k-2$, one has that $\rho(G) < \rho(G')$.*

Proof. Let $\rho = \rho(G)$ be the Harary spectral radius of G and X be the principal eigenvector. By Lemma 2.3, X is positive and can be written as

$$X = (\underbrace{x,\ldots,x}_{s}, \underbrace{y,\ldots,y}_{k-1}, \underbrace{z,\ldots,z}_{2t+1})^T.$$

From the definition of the Harary matrix, we know that

$$RD(G)=\begin{pmatrix}(J-I)_{s\times s} & J_{s\times(k-1)} & J_{s\times(2t+1)}\\ J_{(k-1)\times s} & \frac{1}{2}(J-I)_{(k-1)\times(k-1)} & \frac{1}{2}J_{(k-1)\times(2t+1)}\\ J_{(2t+1)\times s} & \frac{1}{2}J_{(2t+1)\times(k-1)} & (J-I)_{(2t+1)\times(2t+1)}\end{pmatrix}$$

and

$$RD(G')=\begin{pmatrix}(J-I)_{s\times s} & J_{s\times(k-1)} & J_{s\times t} & J_{s\times t} & J_{s\times 1}\\ J_{(k-1)\times s} & \frac{1}{2}(J-I)_{(k-1)\times(k-1)} & J_{(k-1)\times t} & \frac{1}{2}J_{(k-1)\times t} & \frac{1}{2}J_{(k-1)\times 1}\\ J_{t\times s} & J_{t\times(k-1)} & (J-I)_{t\times t} & J_{t\times t} & J_{t\times 1}\\ J_{t\times s} & \frac{1}{2}J_{t\times(k-1)} & J_{t\times t} & \frac{1}{2}(J-I)_{t\times t} & \frac{1}{2}J_{t\times 1}\\ J_{1\times s} & \frac{1}{2}J_{1\times(k-1)} & J_{1\times t} & \frac{1}{2}J_{1\times t} & 0_{1\times 1}.\end{pmatrix}.$$

Thus

$$\begin{aligned}\rho(G')-\rho &\geq X^T(RD(G')-RD(G))X\\ &= t(k-1)yz-\binom{t+1}{2}z^2\\ &= tz((k-1)y-\frac{t+1}{2}z).\end{aligned}\tag{2}$$

As X is the principal eigenvector corresponding to $\rho=\rho(G)$, from Eq. (1), we have

$$\rho y = sx+\frac{k-2}{2}y+\frac{1}{2}(2t+1)z,$$
$$\rho z = sx+\frac{k-1}{2}y+2tz.$$

Then

$$\frac{y}{z}=\frac{2\rho-2t+1}{2\rho+1}.\tag{3}$$

Hence

$$\begin{aligned}(k-1)y-\frac{t+1}{2}z &= (k-1)\frac{2\rho-2t+1}{2\rho+1}z-\frac{t+1}{2}z\\ &= \frac{z}{2(2\rho+1)}(2(2k-t-3)\rho-2(k-1)(2t-1)-(t+1)\\ &= \frac{(2k-t-3)z}{2\rho+1}\left(\rho-\frac{2(k-1)(2t-1)+(t+1)}{2(2k-t-3)}\right).\end{aligned}$$

We now prove that

$$\rho-\frac{2(k-1)(2t-1)+(t+1)}{2(2k-t-3)}>0.$$

Note that K_{s+2t+1} is a subgraph of G. By Corollary 2.2 we have that

$$\rho>\rho(K_{s+2t+1})=s+2t>2t.$$

Hence it is sufficient to prove that

$$\frac{2(k-1)(2t-1)+(t+1)}{2(2k-t-3)}\leq 2t.$$

In fact, it is equivalent to the inequality that $-4t^2+(4k-9)t+2k-3\geq 0$, which obviously holds when $t\leq k-2$. Consequently, we have our conclusion. □

Lemma 3.3. *Let $G=K_s\vee(\overline{K_{k-1}}\cup K_{2t+1})$ with $s\geq 2$, $t\geq 0$, and $G'=K_1\vee(\overline{K_{k-s}}\cup K_{2t+2s-1})$. If $t\geq k-1$, one has that $\rho(G)<\rho(G')$.*

Proof. Let $\rho=\rho(G)$ be the Harary spectral radius of G and X be the principal eigenvector. By Lemma 2.3, X is positive and can be written as

$$X = (\underbrace{x, \ldots, x}_{s}, \underbrace{y, \ldots, y}_{k-1}, \underbrace{z, \ldots, z}_{2t+1})^T.$$

From the definition of the Harary matrix, we know that

$$\begin{aligned} X^T(RD(G') - RD(G))X &= \binom{s-1}{2} y^2 - (s-1)x(k-s)y + (s-1)y(2t+1)z \\ &> (s-1)y((2t+1)z - (k-s)x). \end{aligned}$$

As X is the principal eigenvector corresponding to $\rho = \rho(G)$, from Eq. (1), we have

$$\begin{aligned} \rho x &= (s-1)x + (k-1)y + (2t+1)z, \\ \rho z &= sx + \frac{k-1}{2}y + 2tz. \end{aligned}$$

Then

$$\frac{x}{z} = \frac{2\rho - (2t-1)}{\rho + s + 1} < 2 \tag{4}$$

Hence

$$(2t+1)z - (k-s)x > (2t+1-2(k-s))z = (2t-2k+2s-1)z \geq (2s-3)z > 0.$$

Hence we have that

$$\rho(G') - \rho \geq X^T(RD(G') - RD(G))X > 0.$$

□

A component of a graph G is said to be even (odd) if it has an even (odd) number of vertices. We use $o(G)$ to denote the number of odd components of G. Let G be a graph on n vertices with $\alpha'(G) = p$. With these notations, we may now restate the Tutte–Berge formula,

$$n - 2p = \max\{o(G - X) - |X| : X \subset V(G)\}.$$

Theorem 3.4. *Let G be a graph on n vertices with $\alpha'(G) = p$ which has the maximum Harary spectral radius. Then we have that*

1. *if $p = \lfloor \frac{n}{2} \rfloor$, then $G = K_n$;*
2. *if $1 \leq p \leq \lfloor \frac{n}{3} \rfloor$, then $G = K_p \vee \overline{K_{n-p}}$;*
3. *if $\lfloor \frac{n}{3} \rfloor < p < \lfloor \frac{n}{2} \rfloor$, then $G = K_p \vee \overline{K_{n-p}}$, or $G = K_1 \vee (\overline{K_{n-2p}} \cup K_{2p-1})$.*

Proof. The first assertion is trivial, and so we only need to prove the remaining two assertions. Let X_0 be a vertex subset such that $n - 2p = o(G - X_0) - |X_0|$. For convenience, let $|X_0| = s$ and $o(G - X_0) = k$. Then $n - 2p = k - s$. Since $1 \leq p < \lfloor \frac{n}{2} \rfloor$, we know that $k - s \geq 2$. Hence $k \geq 3$.

If $G - X_0$ has an even component, then by adding an edge to G between a vertex of an even component and a vertex of an odd component of $G - X_0$, we obtain a graph G' with matching number p. From Lemma 2.1, we know that $\rho(G') > \rho(G)$, a contradiction to the assumption that G has the maximum Harary spectral radius. So we know that all the components of $G - X_0$ are odd. Let $G_1, G_2, \ldots, G_k$ be the odd components of $G - X_0$. Similarly, $G_1, G_2, \ldots, G_k$ and the subgraph induced by X_0 are all complete, and every vertex of G_i $(i = 1, \ldots, k)$ is adjacent to every vertex in X_0. Thus $G = K_s \vee (K_{n_1} \cup K_{n_2} \cup \ldots \cup K_{n_k})$, where $n_i = |V(G_i)|$ for $i = 1, 2, \ldots, k$.

First, we claim that $G - X_0$ has at most one odd component whose number of vertices is more than one. Assume without loss of generality that $n_2 \geq n_1 \geq 3$. Let $G' = K_s \vee (K_{n_1-2} \cup K_{n_2+2} \cup \ldots \cup K_{n_k})$. We can easily check that $\alpha(G') = p$. From Lemma 3.1, we know that $\rho(G) < \rho(G')$, a contradiction. Then $G = K_s \vee (\overline{K_{k-1}} \cup K_{2t+1})$, where $s + 2t + k = n$. Since $k - s = n - 2p$, we know that $t + s = p$. By Lemmas 3.2 and 3.3, we know that $s = 1$ or $t = 0$, i,e., $G = K_p \vee \overline{K_{n-p}}$, or $G = K_1 \vee (\overline{K_{n-2p}} \cup K_{2p-1})$. Note that if $1 \leq p \leq \lfloor \frac{n}{3} \rfloor$, one has that $p - 1 \leq n - 2p - 1$. By Lemma 3.2, $EE(K_p \vee \overline{K_{n-p}}) > EE(K_1 \vee (\overline{K_{n-2p}} \cup K_{2p-1}))$. So we have our conclusion. □

Remark. Between $K_p \vee \overline{K_{n-p}}$ and $K_1 \vee (\overline{K_{n-2p}} \cup K_{2p-1})$, we cannot determine which one has larger Harary radius if $\lfloor \frac{n}{3} \rfloor < p < \lfloor \frac{n}{2} \rfloor$. For example, through simple calculations, we have that

$$\rho(K_5 \vee \overline{K_8}) > \rho(K_1 \vee (\overline{K_3} \cup K_9))$$

and

$$\rho(K_5 \vee \overline{K_7}) < \rho(K_1 \vee (\overline{K_2} \cup K_9)).$$

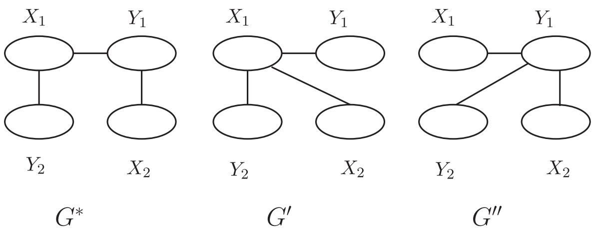

Fig. 1. Graphs G^*, G' and G'' for Lemma 4.4.

4. Bipartite graphs with given matching number

Lemma 4.1 ([3]). *Let K_{n_1,n_2} be a completed bipartite graph with $n = n_1 + n_2$ vertices. One has that*

$$\rho(K_{n_1,n_2}) = \frac{1}{4}(n - 2 + \sqrt{n^2 + 12n_1n_2}).$$

Corollary 4.2.

$$\rho(K_{1,n-1}) < \rho(K_{2,n-2}) < \cdots < \rho(K_{\lfloor \frac{n}{2} \rfloor, \lceil \frac{n}{2} \rceil}). \tag{5}$$

A covering of a graph G is a vertex subset $K \subseteq V(G)$ such that each edge of G has at least one end in the set K. The number of vertices in a minimum covering of a graph G is called the covering number of G and denoted by $\beta(G)$.

Lemma 4.3 (The König–Egerváry theorem, [6,13]). *In any bipartite graph, the number of edges in a maximum matching is equal to the number of vertices in a minimum covering.*

Let $G = G[X, Y] \neq K_{p,n-p}$ be a bipartite graph such that $\alpha'(G) = p$. From Lemma 4.3, we know that $\beta(G) = p$. Let S be a minimum covering of G and $X_1 = S \cap X \neq \emptyset$, $Y_1 = S \cap Y \neq \emptyset$. Set $X_2 = X \setminus X_1$, $Y_2 = Y \setminus Y_1$. We have that $E(X_2, Y_2) = \emptyset$ since S is a covering of G.

Let $G^*[X, Y]$ be a bipartite graph with the same vertex set as G such that $E(G^*) = \{xy : x \in X_1, y \in Y\} \cup \{xy : x \in X_2, y \in Y_1\}$. Obviously, G is a subgraph of G^*. From Lemma 2.1, we know that

$$\rho(G) \le \rho(G^*), \tag{6}$$

where the equality holds if and only if $G = G^*$.

Let

$$G' = G^* - \{uv : u \in X_2, v \in Y_1\} + \{uw : u \in X_2, w \in X_1\}$$

and

$$G'' = G^* - \{uv : u \in X_1, v \in Y_2\} + \{uw : u \in Y_2, w \in Y_1\}.$$

Then we have the following conclusion.

Lemma 4.4. *Let G^*, G' and G'' be the graph defined above (see Fig. 1) with $X_2 \neq \emptyset$ and $Y_2 \neq \emptyset$. Then one has*

$$\rho(G^*) < \rho(G'), \quad \text{or} \quad \rho(G^*) < \rho(G''). \tag{7}$$

Proof. Let $\rho = \rho(G^*)$ be the Harary spectral radius of G^* and X the principal eigenvector. By Lemma 2.3, X is positive and can be written as

$$X = (\underbrace{x_1, \ldots, x_1}_{a}, \underbrace{x_2, \ldots, x_2}_{b}, \underbrace{y_1, \ldots, y_1}_{c}, \underbrace{y_2 \ldots, y_2}_{d})^T,$$

where $a = |X_1|$, $b = |X_2|$, $c = |Y_1|$ and $d = |Y_2|$.

As

$$RD(G^*) = \frac{1}{2}(J - I) + \begin{pmatrix} 0_{a\times a} & \frac{1}{2}J_{a\times b} & J_{a\times c} & J_{a\times d} \\ \frac{1}{2}J_{b\times a} & 0_{b\times b} & J_{b\times c} & \frac{1}{3}J_{b\times d} \\ J_{c\times a} & J_{c\times b} & 0_{c\times c} & \frac{1}{2}J_{c\times d} \\ J_{d\times a} & \frac{1}{3}J_{d\times b} & \frac{1}{2}J_{d\times c} & 0_{d\times d} \end{pmatrix}$$

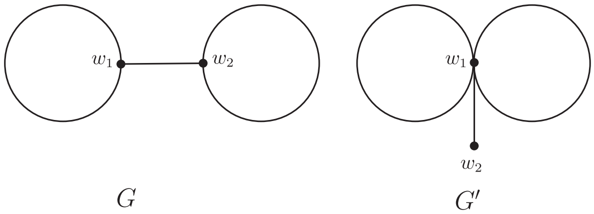

Fig. 2. Graphs G and G' for Lemma 5.1.

and

$$RD(G') = \frac{1}{2}(J - I) + \begin{pmatrix} 0_{a\times a} & J_{a\times b} & J_{a\times c} & J_{a\times d} \\ J_{b\times a} & 0_{b\times b} & \frac{1}{2}J_{b\times c} & \frac{1}{2}J_{b\times d} \\ J_{c\times a} & \frac{1}{2}J_{c\times b} & 0_{c\times c} & \frac{1}{2}J_{c\times d} \\ J_{d\times a} & \frac{1}{2}J_{d\times b} & \frac{1}{2}J_{d\times c} & 0_{d\times d} \end{pmatrix},$$

we have

$$\begin{aligned} X^T(RD(G') - RD(G^*))X &= X^T \begin{pmatrix} 0_{a\times a} & \frac{1}{2}J_{a\times b} & 0_{a\times c} & 0_{a\times d} \\ \frac{1}{2}J_{b\times a} & 0_{b\times b} & -\frac{1}{2}J_{b\times c} & \frac{1}{6}J_{b\times d} \\ 0_{c\times a} & -\frac{1}{2}J_{c\times b} & 0_{c\times c} & 0_{c\times d} \\ 0_{d\times a} & \frac{1}{6}J_{d\times b} & 0_{d\times c} & 0_{d\times d} \end{pmatrix} X \\ &= abx_1x_2 - bcx_2y_1 + \frac{1}{3}bdx_2y_2 \\ &= bx_2(ax_1 - cy_1) + \frac{1}{3}bdx_2y_2. \end{aligned} \tag{8}$$

Similarly, one has that

$$X^T(RD(G'') - RD(G^*))X = dy_2(cy_1 - ax_1) + \frac{1}{3}bdx_2y_2.$$

It is easy to see that either $X^T(RD(G') - RD(G^*))X > 0$ or $X^T(RD(G'') - RD(G^*))X > 0$, i.e., $\rho(G^*) < \rho(G')$ or $\rho(G^*) < \rho(G'')$. □

By (6) and (7), together with Corollary 4.2, it is straightforward to see that

Theorem 4.5. *For any bipartite graph G with matching number p and $G \neq K_{p,n-p}$, one has that $\rho(G) < \rho(K_{p,n-p})$.*

5. Graphs with given number of cut edges

Lemma 5.1. *Let G be a graph with a cut edge $e = w_1w_2$, and G' be the graph obtained from G by contracting edge e and adding a pendent edge attaching at the contracting vertex (see Fig. 2). If $d_G(w_i) \geq 2$ for $i = 1, 2$, we have that $\rho(G') > \rho(G)$.*

Proof. Let $\rho(G)$ be the Harary spectral radius of G and X the corresponding principal eigenvector. Without loss of generality, we assume that $x_{w_1} \geq x_{w_2}$. We denote the contracting vertex by w_1, and the pendant edge by w_1w_2. Let G_i be the component of $G - e$ that contains w_i for $i = 1, 2$. Let $V_1' = V(G_1) \setminus \{w_1\}$ and $V_2' = V(G_2) \setminus \{w_2\}$. For any two vertices u and v, we have that

$$d_{G'}(u, v) = \begin{cases} d_G(u, v) - 1, & \text{if } u \in V(G_1) \text{ and } v \in V_2', \\ d_G(u, v) + 1, & \text{if } u = w_2 \text{ and } v \in V_2', \\ d_G(u, v), & \text{otherwise.} \end{cases}$$

Let

$$A = \sum_{w_1 \in V_1', w_2 \in V_2'} \left(\frac{1}{d_{G'}(w_1, w_2)} - \frac{1}{d_G(w_1, w_2)} \right) x_{w_1}x_{w_2} > 0.$$

From the definition of the Harary matrix, we know that

$$\rho(G') - \rho(G) \geq X^TRD(G')X - X^TRD(G))X$$

$$
\begin{aligned}
&= \sum_{u,v\in V(G)} \left(\frac{1}{d_{G'}(u,v)} - \frac{1}{d_G(u,v)}\right)x_u x_v \\
&= 2A + 2\sum_{u=w_1, v\in V_2'} \left(\frac{1}{d_{G'}(u,v)} - \frac{1}{d_G(u,v)}\right)x_u x_v + 2\sum_{u=w_2, v\in V_2'} \left(\frac{1}{d_{G'}(u,v)} - \frac{1}{d_G(u,v)}\right)x_u x_v \\
&= 2A + 2\sum_{v\in V_2'} x_v \left(\frac{x_{w_1}}{d_G(w_1,v)(d_G(w_1,v)-1)} - \frac{x_{w_2}}{d_G(w_2,v)(d_G(w_2,v)+1)}\right) \\
&= 2A + 2(x_{w_1} - x_{w_2})\sum_{v\in V_2'} \frac{1}{d_G(w_1,v)(d_G(w_1,v)-1)} x_v \\
&\geq 2A > 0.
\end{aligned}
$$

Note that the last equality holds since $d_G(w_1, v) = d_G(w_2, v) + 1$ for any $v \in V_2'$. Hence we have our conclusion. □

Assume that $r_1, r_2, \ldots, r_s$ are positive integers, and $s \leq t$. Let $K_t(r_1, r_2, \ldots, r_s)$ be the graph that is obtained from K_t with $V(K_t) = \{v_1, v_2, \ldots, v_t\}$ by attaching r_i pendant edges to vertex v_i for $1 \leq i \leq s$.

Lemma 5.2. *Let $G = K_t(r_1, r_2, \ldots, r_s)$ and $G' = K_t(r_1 + r_2 + \cdots + r_s)$. Then $\rho(G') > \rho(G)$.*

Proof. Let $\rho(G)$ be the Harary spectral radius of G and X the corresponding principal eigenvector. Let R_i be set of pendant vertices that is adjacent to v_i in G. From Lemma 2.3, we can suppose that $x_u = a_i$ for all $u \in R_i$ $(1 \leq i \leq s)$. Without loss of generality, assume that $x_{v_1} \geq x_{v_i}$ for $2 \leq i \leq s$. Let $G'' = G - \{v_2 w : w \in R_2\} + \{v_1 w : w \in R_2\}$, that is, $G'' = K_t(r_1 + r_2, r_3, \ldots, r_s)$. For any two vertices u and v, if neither u nor v belongs to R_2, we know that $d_G(u, v) = d_{G''}(u, v)$; If both u and v belong to R_2, we can also get $d_G(u, v) = d_{G''}(u, v)$. If exactly one of u and v belongs to R_2, say $u \in R_2$, we have the following equation:

$$
d_{G''}(u,v) = \begin{cases} d_G(u,v) - 1 = 2, & \text{if } v \in R_1, \\ d_G(u,v) - 1 = 1, & \text{if } v = v_1 \\ d_G(u,v) + 1 = 2, & \text{if } v = v_2, \\ d_G(u,v), & \text{otherwise.} \end{cases}
$$

From the definition of the Harary matrix, we know that

$$
\begin{aligned}
\rho(G'') - \rho(G) &\geq X^T RD(G'')X - X^T RD(G)X \\
&= \sum_{u,v\in V(G)} \left(\frac{1}{d_{G''}(u,v)} - \frac{1}{d_G(u,v)}\right)x_u x_v \\
&= 2\sum_{u\in R_2, v\notin R_2} \left(\frac{1}{d_{G''}(u,v)} - \frac{1}{d_G(u,v)}\right)x_u x_v \\
&= 2r_2 a_2 \left(\sum_{v\in R_1}\left(\frac{1}{2} - \frac{1}{3}\right)x_v + \left(1 - \frac{1}{2}\right)x_{v_1} + \left(\frac{1}{2} - 1\right)x_{v_2}\right) \\
&= \frac{1}{3} r_1 r_2 a_1 a_2 + r_2 a_2 (x_{v_1} - x_{v_2}) \\
&> 0.
\end{aligned}
$$

By repeating this process until all the pendant edges have a common end, we can obtain our conclusion. □

From Lemmas 2.1, 5.1 and 5.2, we have the following theorem.

Theorem 5.3. *Let G be a graph on n vertices with p cut edges which has the maximum Harary spectral radius, then $G = K_{n-p}(p)$.*

Corollary 5.4. *The n-vertex star S_n is the unique tree on n vertices which has the maximum Harary spectral radius.*

Acknowledgment

The authors would like to thank the editor and reviewers for helpful comments and suggestions.

References

[1] M. Aouchiche, P. Hansen, Distance spectra of graphs: a survey, Linear Algebra Appl. 458 (2014) 301–386.
[2] J.A. Bondy, U.S.R. Murty, Graph Theory, Springer, New York, 2008.
[3] Z. Cui, B. Liu, On Harary matrix, Harary index and Harary energy, MATCH Commun. Math. Comput. Chem. 68 (2012) 815–823.
[4] K.C. Das, Maximum eigenvalues of the reciprocal distance matrix, J. Math. Chem. 47 (2010) 21–28.

[5] J. Devillers, A.T. Balaban (Eds.), Topological Indices and Related Descriptors in QSAR and QSPR, Gordon and Breach, Amsterdam, 1999.
[6] E. Egerváry, On combinatorial properties of matrices, Mat. Lapok. 38 (1931) 16–28 (Hungarian with German summary).
[7] 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.
[8] I. Gutman, M. Medeleanu, On the structure-dependence of the largest eigenvalue of the distance matrix of an alkane, Indian J. Chem. 37A (1998) 569–573.
[9] X. Guo, D.J. Klein, W. Yan, Y.-N. Yeh, Hyper-Wiener vector, wiener matrix sequence, and wiener polynomial sequence of a graph, Int. J. Quantum. Chem. 106 (2006) 1756–1761.
[10] 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.
[11] O. Ivanciuc, T. Ivanciuc, A.T. Balaban, Quantitative structure–property relationship evaluation of structural descriptors derived from the distance and reverse wiener matrices, Internet Eletron. J. Mol. Des. 1 (2002) 467–487.
[12] D.J.z. c, A.M. Cević, S. Nikolić, N. Trinajstić, Graph Theoretical Matrices in Chemistry, Mathematical Chemistry Monographs No. 3, University of Kragujevac, Kragujevac, 2007.
[13] D. König, Graphs and matrices, Mat. Fiz. Lapok 38 (1931) 116–119 Hungarian.
[14] Z. Liu, On spectral radius of the distance matrix, Appl. Anal. Discrete Math. 4 (2010) 269–277.
[15] Z. Mihalić, D. Veljan, D. Amić, S. Nikolić, D.P. Sić, N. Trinajstić, The distance matrix in chemistry, J. Math. Chem. 11 (1992) 223–258.
[16] R. Todeschini, V. Consonni, Handbook of Molecular Descriptors, Wiley-VCH, Weinheim, 2000.
[17] K. Xu, M. Liu, K.C. Das, I. Gutman, B. Furtula, A survey on graphs extremal with respect to distance-based topological indices, MATCH Commu. Math. Comput. Chem. 71 (2014) 461–508.
[18] B. Zhou, N. Trinajstć, Maximum eigenvalues of the reciprocal distance matrix and the reverse wiener matrix, Int. J. Quantum Chem. 108 (2008) 858–864.