

On the Maximum Harary Spectral Radius of Graphs with Given Matching Number

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Abstract—The Harary spectral radius was proved to be able to produce fair QSPR models for the boiling points, molar heat capacities, vaporization enthalpies, refractive indices and densities for C₆-C₁₀ alkanes. Hence this structure-descriptor has recently attracted attention of chemists and mathematicians. [Ars Combin. 131 (2017) 23] and [Appl. Math. Comput. 266 (2015) 937] considered the maximum Harary spectral radius of graphs with given matching number. However, the results are wrong or incomplete. This paper gives an almost complete solution to the problem.

Keywords—Harary matrix; spectral radius; matching number; extremal graph

I. INTRODUCTION

We consider non-trivial connected simple graphs only. Such a graph will be denoted by $G = (V, E)$, where $V = \{v_1, v_2, \dots, v_n\}$ and $E = E(G)$ are the vertex set and edge set of G , respectively. \bar{G} will denote the complement of G . Let $G_1 \cup G_2$ be the vertex-disjoint union of the graphs G_1 and G_2 , and $G_1 \vee G_2$ the graph obtained from $G_1 \cup G_2$ by joining each vertex of G_1 to each vertex of G_2 .

A matching of G is a set of pairwise non-adjacent edges. A maximum matching is one which contains as many edges as possible. The cardinality of a maximum matching of G is called the matching number of G .

The Harary matrix $RD(G)$ of G , which is also known as the reciprocal distance matrix [1], is an $n \times n$ matrix whose (i, j) -entry RD_{ij} is equal to $1/d_{ij}$ if $i \neq j$ and 0 otherwise, where d_{ij} is the distance between v_i and v_j in G . Since $RD(G)$ is non-negative and symmetric, its eigenvalues are all real. The spectral radius (the largest eigenvalue) of $RD(G)$, denoted by $\rho(G)$, is called the Harary spectral radius of G . The Harary index of G is defined as $\sum_{i < j} RD_{ij}$, and the Harary energy of G is the sum of the absolute values of all eigenvalues of $RD(G)$.

Ivanciuc et al. [2] showed that, the Harary spectral radius is able to produce fair quantitative structure - property relationships (QSPR) models for the boiling points, molar heat capacities, vaporization enthalpies, refractive indices and densities for C₆-C₁₀ alkanes. Hence this structure-descriptor has

recently attracted attention of chemists and mathematicians. The lower and upper bounds of the Harary spectral radius of the Harary matrix, and the Nordhaus-Gaddum-type results for it were obtained in [3, 4]. Cui and Liu [5] proposed some more results about the eigenvalues of Harary matrices; also, they got some bounds of the Harary energy. Some lower and upper bounds for the Harary energy of connected (n, m) -graphs were obtained in [6]. One can also refer to the book [7] for some properties and applications of Harary index and its variants.

Zhu et al. [8] considered the maximum Harary spectral radius of graphs with given matching number p , and claimed that, the extremal graph is $G = K_1 \vee (K_{2p-1} \cup \overline{K_{n-2p}})$ if $p < \lfloor n/2 \rfloor$, where K_a denotes the complete graph of order a . However, the result is wrong. Independently, Huang et al. [9] considered the same problem, and proved the following result.

Theorem 1.1 [9]. Let G be a graph on n vertices with matching number p which has the maximum Harary spectral radius. Then

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

Hence, for the case $\lfloor n/3 \rfloor < p < \lfloor n/2 \rfloor$ the extremal graph has not been characterized completely. In the rest of this paper, we let $G_1 = K_1 \vee (K_{2p-1} \cup \overline{K_{n-2p}})$ and $G_2 = K_p \vee \overline{K_{n-p}}$. For completeness, one needs to know when $\rho(G_1) > \rho(G_2)$ holds. In Section II, we will prove that, $\rho(G_1) > \rho(G_2)$ if $p > p_0(n) = (24n + 9 - \sqrt{48n^2 - 8n - 7})/44$.

II. MAIN RESULTS

Since $RD(G)$ is real, non-negative, and irreducible, from the Perron-Frobenius theorem, $\rho(G)$ is positive, simple, and there is a unique positive unit eigenvector X corresponding to $\rho(G)$, which is called the Perron vector of $RD(G)$. That is,

$\rho(G) = \max_{\|Y\|=1} Y^T R D(G) Y = X^T R D(G) X$. Moreover, we have $\rho(G)X = R D(G)X$.

Let $\rho_1 = \rho(G_1)$, and $\rho_2 = \rho(G_2)$. Let $J_{k \times l}$ be the $k \times l$ matrix whose entries are all equal to 1, and I_k the $k \times k$ unit matrix. It is easily seen that,

$$R D(G_1) = \begin{pmatrix} (J - I)_{(2p-1) \times (2p-1)} & J_{(2p-1) \times 1} & \frac{1}{2} J_{(2p-1) \times (n-2p)} \\ J_{1 \times (2p-1)} & 0_{1 \times 1} & J_{1 \times (n-2p)} \\ \frac{1}{2} J_{(n-2p) \times (2p-1)} & J_{(n-2p) \times 1} & \frac{1}{2} (J - I)_{(n-2p) \times (n-2p)} \end{pmatrix},$$

and

$$R D(G_2) = \begin{pmatrix} (J - I)_{p \times p} & J_{p \times (n-p)} \\ J_{(n-p) \times p} & \frac{1}{2} (J - I)_{(n-p) \times (n-p)} \end{pmatrix}.$$

Let

$$A = \begin{pmatrix} (J - I)_{2p \times 2p} & \frac{1}{2} J_{2p \times (n-2p)} \\ \frac{1}{2} J_{(n-2p) \times 2p} & \frac{1}{2} (J - I)_{(n-2p) \times (n-2p)} \end{pmatrix},$$

and $\rho_3 = \rho(A)$. Since

$$B = R D(G_1) - A = \begin{pmatrix} 0_{(2p-1) \times (2p-1)} & 0_{(2p-1) \times 1} & 0_{(2p-1) \times (n-2p)} \\ 0_{1 \times (2p-1)} & 0_{1 \times 1} & \frac{1}{2} J_{1 \times (n-2p)} \\ 0_{(n-2p) \times (2p-1)} & \frac{1}{2} J_{(n-2p) \times 1} & 0_{(n-2p) \times (n-2p)} \end{pmatrix}$$

is non-negative, $\rho_1 > \rho_3$ holds immediately from the Perron-Frobenius theorem.

To compare ρ_3 and ρ_2 , we will use a novel technique that involves comparing the largest roots of two certain polynomials. Let $f(x)$ be a polynomial, $\deg(f)$ and $\lambda_1(f)$ will denote the degree and the largest root of $f(x)$, respectively.

Lemma 2.1. Let $f(x)$ and $g(x)$ be two monic polynomials with real roots, such that $\deg(f) \geq \deg(g)$ and $f(x) = q(x)g(x) + ax + b$, where $a \neq 0$, b are two real numbers, $q(x)$ is a monic polynomial with $\lambda_1(q) < \lambda_1(g)$, and $f(x)$, $g(x)$ increase monotonically in $[-b/a, +\infty)$. Then we have

(1) If $a > 0$, then $\lambda_1(f) \geq \lambda_1(g)$ iff $g(-b/a) \geq 0$, with the equality iff $g(-b/a) = 0$.

(2) If $a < 0$, then $\lambda_1(f) \geq \lambda_1(g)$ iff $g(-b/a) \leq 0$, with the equality iff $g(-b/a) = 0$.

Proof. (1) If $g(-b/a) \geq 0$, then $g(x) > 0$ for $x > -b/a$, since $g(x)$ increases monotonically in $[-b/a, +\infty)$. Hence $\lambda_1(g) \leq -b/a$, and $f(\lambda_1(g)) = a\lambda_1(g) + b \leq 0$, which implies $\lambda_1(f) \geq \lambda_1(g)$, with the equality iff $f(-b/a) = 0$.

Conversely, if $g(-b/a) < 0$, then $\lambda_1(g) > -b/a$. Since $\lambda_1(q) < \lambda_1(g)$, $q(x) > 0$ for $x \geq \lambda_1(g)$. Hence we have $f(x) = q(x)g(x) + ax + b > 0$ for all $x \geq \lambda_1(g)$, which implies $\lambda_1(f) < \lambda_1(g)$.

(2) Analogously to Case (1). ■

Lemma 2.2. $\rho_3 \geq \rho_2$ iff $p \geq p_0(n)$, with the equality iff $p_0(n)$ is an integer and $p = p_0(n)$.

Proof. Let $X = (x_1^{2p}, x_2^{n-2p})'$ be the Perron vectors of A , where z^k denotes k consecutive z 's. From $\rho_3 X = AX$ we have

$$\begin{cases} \rho_3 x_1 = (2p-1)x_1 + \frac{1}{2}(n-2p)x_2 \\ \rho_3 x_2 = px_1 + \frac{1}{2}(n-2p-1)x_2 \end{cases}$$

$$\Rightarrow \begin{cases} 2(\rho_3 - 2p + 1)x_1 = (n-2p)x_2 \\ (2\rho_3 - n + 2p + 1)x_2 = 2px_1 \end{cases}$$

$$\Rightarrow \frac{2x_1}{x_2} = \frac{n-2p}{\rho_3 - (2p-1)} = \frac{2\rho_3 - (n-2p-1)}{p}$$

$$\Rightarrow 2\rho_3^2 - (n+2p-3)\rho_3 + (pn-2p^2-n+1) = 0.$$

Since A is nonnegative and irreducible, ρ_3 is bounded by the minimum and maximum row sums of A . Noting $p \leq n/2$, we immediately have $\rho_3 \geq (n-1)/2 > (n+2p-3)/4$. Hence ρ_3 is the larger (real) root of the quadratic function $f(x) = x^2 - (n+2p-3)x/2 + (pn-2p^2-n+1)/2$.

Similarly, ρ_2 is the larger root of the quadratic function $g(x) = x^2 - (n+p-3)x/2 + (p^2-pn-n+1)/2$.

Let $x_0 = 2n-3p$ and $r(x) = p(x_0 - x)/2$. Then $f(x) = g(x) + r(x)$. Since $p < n/2$, it is easily confirmed that, $x_0 > (n+2p-3)/4 > (n+p-3)/4$. Hence $f(x)$ and $g(x)$ increase monotonically in $[x_0, +\infty)$. From Lemma 2.1 (2) we have $\rho_3 \geq \rho_2$ iff $g(x_0) \leq 0$, with the equality iff $g(x_0) = 0$. By elementary computations we have

$$g(x_0) \leq 0 \Leftrightarrow x_0^2 - (n+p-3)x_0/2 + (p^2-pn-n+1)/2 \leq 0$$

$$\Leftrightarrow 22p^2 - (24n+9)p + 6n^2 + 5n + 1 \leq 0$$

$$\Leftrightarrow p \geq p_0(n) = (24n+9 - \sqrt{48n^2 - 8n - 7}) / 44.$$

The proof is thus completed. ■

Theorem 2.3. If $p > p_0(n)$, then $\rho_1 > \rho_2$.

Proof. Immediate from $\rho_1 > \rho_3$ and Lemma 2.2. ■

III. FURTHER DISCUSSIONS

Theorem 2.3 partially solves the comparison between $\rho_1 = \rho(K_1 \vee (K_{2p-1} \cup K_{n-2p}))$ and $\rho_2 = \rho(K_p \vee K_{n-p})$. However, the case $\lfloor n/3 \rfloor < p < p_0(n)$ remains unknown. Naturally, we propose the following conjecture.

Conjecture 3.1. There exists a positive integer $p_1(n)$ with $\lceil p_0(n) \rceil - p_1(n) \leq 1$ such that, $\rho_1 \geq \rho_2$ iff $p \geq p_1(n)$, with the equality iff $p = p_1(n)$.

To support the above conjecture, we conducted a numerical experiment, which confirms the conjecture for $n \leq 1500$.

To prove or disprove Conjecture 3.1, one may need to estimate the gap $\rho_1 - \rho_3$ precisely. However, at the present we only have the following result, which is quite trivial.

Lemma 3.2. $\rho_1 - \rho_3 \leq (n-2p)/2$, and $\rho_1 - \rho_3 < n/6$ if $p > n/3$.

Proof. Since

$$B = RD(G_1) - A = \begin{pmatrix} 0_{(2p-1) \times (2p-1)} & 0_{(2p-1) \times 1} & 0_{(2p-1) \times (n-2p)} \\ 0_{1 \times (2p-1)} & 0_{1 \times 1} & \frac{1}{2} J_{1 \times (n-2p)} \\ 0_{(n-2p) \times (2p-1)} & \frac{1}{2} J_{(n-2p) \times 1} & 0_{(n-2p) \times (n-2p)} \end{pmatrix}$$

is nonnegative and irreducible, $\rho(B)$ is bounded by the minimum and maximum row sums of B , hence $\rho(B) \leq (n-2p)/2$. From the Courant-Weyl inequality [10] we have $\rho_1 - \rho_3 \leq \rho(B) \leq (n-2p)/2$, and $\rho_1 - \rho_3 < n/6$ if $p > n/3$. ■

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