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Randić Spectral Radius and Randić Energy

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HAPPY 80-th BIRTHDAY PROFESSOR RANDIĆ

Abstract

Let G be a simple connected graph with n vertices and let d_i be the degree of its i-th vertex. The Randić matrix of G is the square matrix of order n whose (i, j)-entry is equal to $1/\sqrt{d_i\,d_j}$ if the i-th and j-th vertex of G are adjacent, and zero otherwise. The Randić eigenvalues are the eigenvalues of the Randić matrix. The greatest Randić eigenvalue is the Randić spectral radius of G. The Randić energy is the sum of the absolute values of the Randić eigenvalues. Lower bounds for Randić spectral radius and an upper bound for Randić energy are obtained. Graphs for which these bounds are best possible are characterized.

1 Introduction

Let G be a simple connected graph on the vertex set $V(G) = \{v_1, v_2, \ldots, v_n\}$. If two vertices v_i and v_j of G are adjacent, then we use the notation $v_i \sim v_j$. For $v_i \in V(G)$, the degree of the vertex v_i, denoted by d_i, is the number of the vertices adjacent to v_i. Let $\mathbf{A}(G)$ be adjacency matrix of G and $\lambda_1, \lambda_2, \ldots, \lambda_n$ its eigenvalues. These are said to be the eigenvalues of the graph G and to form its spectrum [1, 2].

The energy $E(G)$ of a graph G is defined as the sum of the absolute values of its eigenvalues:

$$E = E(G) = \sum_{i=1}^{n} |\lambda_i| \,. \tag{1}$$

Details and more information on graph energy can be found in the reviews [3–6] and the recent papers [7–13].

The *Randić matrix* of G is the $n \times n$ matrix $\mathbf{R} = \mathbf{R}(G) = \|R_{ij}\|$ defined via

$$R_{ij} = \begin{cases} \dfrac{1}{\sqrt{d_i\, d_j}} & \text{if } v_i \sim v_j \\ 0 & \text{otherwise} \end{cases} \,.$$

This matrix was earlier studied [14–17] in connection with the Randić index. Its role in the Laplacian spectral theory was clarified in the recent article [18].

The Randić eigenvalues $\rho_1, \rho_2, \ldots, \rho_n$ of a graph G are the eigenvalues of its Randić matrix $\mathbf{R}$. Since $\mathbf{R}$ is a real symmetric matrix, all its eigenvalues are real numbers and thus we can order them so that $\rho_1 \geq \rho_2 \geq \cdots \geq \rho_n$. The greatest eigenvalue ρ_1 will be called the *Randić spectral radius* of the graph G.

The concept of *Randić energy* of a graph G, denoted by $RE(G)$, was introduced in [18] as:

$$RE = RE(G) = \sum_{i=1}^{n} |\rho_i|$$

and was conceived in full analogy with the ordinary graph energy, Eq. (1). In [18] some bounds for RE were obtained.

In this paper, we obtain lower bounds for ρ_1 and an upper bound for RE. We then characterize graphs for which these bounds are best possible.

In the subsequent section we give a few definitions that will be needed for the formulation and proof of our main results.

2 Auxiliary definitions

- Let G be a graph with vertex set $V(G) = \{v_1, v_2, \ldots, v_n\}$ and Randić matrix $\mathbf{R}$. Then the *Randić degree* of v_i, denoted by R_i, is given by

$$R_i = \sum_{j=1}^{n} R_{ij} \ .$$

- Let G be a graph with vertex set $V(G) = \{v_1, v_2, \ldots, v_n\}$ and Randić matrix $\mathbf{R}$. Let its Randić degree sequence be $\{R_1, R_2, \ldots, R_n\}$. Then the *second Randić degree* of v_i, denoted by S_i, is given by

$$S_i = \sum_{j=1}^{n} R_{ij} \, R_j \ .$$

- Let G be a graph with Randić degree sequence $\{R_1, R_2, \ldots, R_n\}$. Then G is a *k-Randić regular* if $R_i = k$, for all i.

- Let G be a graph with Randić degree sequence $\{R_1, R_2, \ldots, R_n\}$ and second Randić degree sequence $\{S_1, S_2, \ldots, S_n\}$. Then G is *pseudo k-Randić regular* if $S_i/R_i = k$ for all i.

- Let G be a graph with the Randić matrix $\mathbf{R}$. Then the *Randić index* of G, denoted by $R(G)$, is given by

$$R(G) = \frac{1}{2} \sum_{i=1}^{n} R_i \ .$$

  Although well known, we repeat that this molecular structure descriptor was invented by Milan Randić in 1976 [19]; for details see the books [20–22], reviews [23–26], and recent papers [27–29].

3 Lower bounds for Randić spectral radius

The following lemma is important for finding the best lower bound for Randić spectral radius ρ_1.

Lemma 1. Let G be a graph with n vertices. Then

$$\sum_{i=1}^{n} S_i = \sum_{i=1}^{n} R_i^2 \ .$$

Proof. By the definitions given in the preceding section,

$$R_i = \sum_{i \sim j} \frac{1}{\sqrt{d_i\, d_j}} \qquad \text{and} \qquad S_i = \sum_{i \sim j} \frac{1}{\sqrt{d_i\, d_j}}\, R_j \ .$$

By the associativity of matrix multiplication, we obtain

$$\begin{aligned} S_1 + S_2 + \cdots + S_n &= (1,1,\ldots,1)\,(\mathbf{R}\,(R_1, R_2, \ldots, R_n)^T) \\ &= ((1,1,\ldots,1)\,\mathbf{R})\,(R_1, R_2, \ldots, R_n)^T \\ &= R_1^2 + R_2^2 + \cdots + R_n^2 \ . \end{aligned}$$

Hence the result. ■

Theorem 1. Let G be a simple connected graph with n vertices and let $R(G)$ be its Randić index. Then

$$\rho_1 \geq \frac{2R(G)}{n} \ . \tag{2}$$

The equality holds in (2) if and only if G is Randić regular.

Proof is analogous to what was earlier used in [30]. Let $X = \frac{1}{\sqrt{n}}\,(1,1,\ldots,1)^T$ be a unit n-vector. By applying the Rayleigh principle to Randić matrix $\mathbf{R}$ of G we obtain

$$\begin{aligned} \rho_1 &\geq \frac{X^T \mathbf{R} X}{X^T X} = \frac{\frac{1}{\sqrt{n}}\,(R_1, R_2, \ldots, R_n)\,\frac{1}{\sqrt{n}}\,(1,1,\ldots,1)^T}{1} \\ &= \frac{1}{n} \sum_{i=1}^{n} R_i = \frac{2R(G)}{n} \ . \end{aligned}$$

Suppose now that G is Randić regular. The sum of each rows of $\mathbf{R}$ is equal to a constant, say k. Clearly $2R(G) = nk$. Then, by the Perron–Frobenius theorem, k is the greatest and simple eigenvalue of $\mathbf{R}$. Thus $\rho_1 = k = 2R(G)/n$. Hence we get the equality in (2), as required. Conversely if the equality holds, then X is the eigenvector corresponding to ρ_1 i. e., $\mathbf{R}\,X = \rho_1\,X$. This implies that $R_i = \rho_1$ holds for all i. ■

Theorem 2. Let G be a simple connected graph on the vertex set $V(G) = \{v_1, v_2, \ldots, v_n\}$ and let R_i be the Randić degree of v_i. Then

$$\rho_1 \geq \sqrt{\frac{1}{n} \sum_{i=1}^{n} R_i^2}\,. \tag{3}$$

The equality holds in (3) if and only if G is Randić regular.

Proof. Let $\mathbf{R}$ be the Randić matrix of G and let $X = (x_1, x_2, \ldots, x_n)^T$ be the unit positive Perron eigenvector of $\mathbf{R}$ corresponding to ρ_1. We take

$$C = \frac{1}{\sqrt{n}}\,(1, 1, \ldots, 1)^T\,.$$

Since C is a unit positive vector, we have

$$\rho_1 = \rho_1(\mathbf{R}) = \sqrt{\rho_1(\mathbf{R}^2)} = \sqrt{X^T\,\mathbf{R}^2\,X} \geq \sqrt{C^T\,\mathbf{R}^2\,C}\,.$$

Now

$$\mathbf{R}\,C = \frac{1}{\sqrt{n}}\,\mathbf{R}\,(1, 1, \ldots, 1)^T = \frac{1}{\sqrt{n}}\,(R_1, R_2, \ldots, R_n)^T\,.$$

Therefore

$$\rho_1 \geq \sqrt{C^T\,\mathbf{R}^2\,C} = \sqrt{\frac{1}{n} \sum_{i=1}^{n} R_i^2}\,.$$

Hence we arrived at inequality (3).

Consider now the case of equality. Suppose that G is Randić regular. Then $R_i = k$ for all i, and hence, by the Perron–Frobenius theorem, k is the greatest and simple eigenvalue of $\mathbf{R}$. Then

$$\rho_1 = k = \sqrt{\frac{nk^2}{n}} = \sqrt{\frac{1}{n} \sum_{i=1}^{n} R_i^2}$$

and hence the equality holds in (3). Conversely, if the equality holds in (3), then C is the eigenvector corresponding to ρ_1. Then as in the proof of Theorem 1, we conclude that G is Randić regular. ■

In order to obtain a better lower bound for the Randić spectral radius we define the sequence $L_i^{(1)}, L_i^{(2)}, \ldots, L_i^{(p)}, \ldots$, such that $L_i^{(1)} = R_i^\alpha$ whereas for $p \geq 2$,

$$L_i^{(p)} = \sum_{i \sim j} \frac{1}{\sqrt{d_i\,d_j}}\,L_j^{(p-1)}\,.$$

In these formulas, $\alpha \in \mathbb{R}$.

Theorem 3. Let G be a simple connected graph, α be a real number, and p be an integer. Then

$$\rho_1 \geq \sqrt{\frac{\sum_{i=1}^{n} \left(L_i^{(p+1)}\right)^2}{\sum_{i=1}^{n} \left(L_i^{(p)}\right)^2}} \,. \tag{4}$$

Equality in (4) holds if and only if

$$\frac{L_1^{(p+1)}}{L_1^{(p)}} = \frac{L_2^{(p+1)}}{L_2^{(p)}} = \cdots = \frac{L_n^{(p+1)}}{L_n^{(p)}} \,.$$

Proof. Let $X = (x_1, x_{2,\ldots,} x_n)^T$ be the unit positive Perron eigenvector of $\mathbf{R}$ corresponding to ρ_1. In this case, let us take

$$C = \frac{1}{\sqrt{\sum_{i=1}^{n} \left(L_i^{(p)}\right)^2}} \left(L_1^{(p)}, L_2^{(p)}, \ldots, L_n^{(p)}\right)^T .$$

As previously, since C is a unit positive vector, we have

$$\rho_1 = \rho_1(\mathbf{R}) = \sqrt{\rho_1(\mathbf{R}^2)} = \sqrt{X^T\, \mathbf{R}^2\, X} \geq \sqrt{C^T\, \mathbf{R}^2\, C} \,. \tag{5}$$

Furthermore

$$\begin{aligned} \mathbf{R}\, C &= \frac{1}{\sqrt{\sum_{i=1}^{n} \left(L_i^{(p)}\right)^2}} \left(\sum_{1\sim j} \frac{1}{\sqrt{d_1\, d_j}}\, L_j^{(p)}, \sum_{2\sim j} \frac{1}{\sqrt{d_2\, d_j}}\, L_j^{(p)}, \ldots, \sum_{n\sim j} \frac{1}{\sqrt{d_n\, d_j}}\, L_j^{(p)} \right)^T \\ &= \frac{1}{\sqrt{\sum_{i=1}^{n} \left(L_i^{(p)}\right)^2}} \left(L_1^{(p+1)}, L_2^{(p+1)}, \ldots, L_n^{(p+1)}\right)^T . \end{aligned}$$

Then we obtain

$$\rho_1 \geq \sqrt{C^T\, \mathbf{R}^2\, C} = \sqrt{\frac{\sum_{i=1}^{n} \left(L_i^{(p+1)}\right)^2}{\sum_{i=1}^{n} \left(L_i^{(p)}\right)^2}} \,.$$

Suppose now that the equality holds in (4). From inequality (5), we get that C is an eigenvector corresponding to ρ_1. Then $\mathbf{R}\, C = \rho_1\, C$ which implies $L_i^{(p+1)}/L_i^{(p)} = \rho_1$ for all i.

Conversely, let
$$\frac{L_1^{(p+1)}}{L_1^{(p)}} = \frac{L_2^{(p+1)}}{L_2^{(p)}} = \cdots = \frac{L_n^{(p+1)}}{L_n^{(p)}} = k \ .$$
Then $\mathbf{R}\,C = k\,C$, that is, C is an eigenvector corresponding to k. Hence we get $\rho_1 = k$. Thus the equality holds in (4), as claimed. ■

By setting $\alpha = 1$ and $p = 1$ in (4), we directly get:

Corollary 1. Let G be a simple connected graph with Randić degree sequence $\{R_1, R_2, \ldots, R_n\}$ and second Randić degree sequence $\{S_1, S_2, \ldots, S_n\}$. Then
$$\rho_1 \geq \sqrt{\frac{\sum_{i=1}^{n} S_i^2}{\sum_{i=1}^{n} R_i^2}} \ . \tag{6}$$
Equality holds if and only if G is pseudo k-Randić regular, for some k.

Theorem 4. The lower bound for ρ_1 given in (4) improves the lower bounds given in (2), (3), and (6).

Proof. For any fixed values $\alpha \in \mathbb{R}$ and $p \in \mathbb{N}$,
$$\rho_1 \geq \sqrt{\frac{\sum_{i=1}^{n} \left(L_i^{(p+1)}\right)^2}{\sum_{i=1}^{n} \left(L_i^{(p)}\right)^2}} \geq \sqrt{\frac{\sum_{i=1}^{n} S_i^2}{\sum_{i=1}^{n} R_i^2}} \ .$$
By the Cauchy–Schwarz inequality and Lemma 1 we have
$$\sqrt{\frac{\sum_{i=1}^{n} S_i^2}{\sum_{i=1}^{n} R_i^2}} \geq \sqrt{\frac{\left(\sum_{i=1}^{n} S_i\right)^2}{n\sum_{i=1}^{n} R_i^2}} = \sqrt{\frac{\left(\sum_{i=1}^{n} R_i^2\right)^2}{n\sum_{i=1}^{n} R_i^2}}$$
$$= \sqrt{\frac{\sum_{i=1}^{n} R_i^2}{n}} \geq \sqrt{\frac{\left(\sum_{i=1}^{n} R_i\right)^2}{n^2}} = \frac{2R(G)}{n} \ .$$
Hence the result. ■

Lemma 2. A simple connected graph G has two distinct Randić eigenvalues if and only if G is complete.

Proof is similar to that of Lemma 2 in [7]. Let G be a simple connected graph with Randić matrix $\mathbf{R}$. We suppose that G has exactly two distinct Randić eigenvalues. Let these be $\rho_1 > \rho_2$. Since G is connected, $\mathbf{R}$ is irreducible and by the Perron–Frobenius theorem, ρ_1 is the greatest and simple eigenvalue of $\mathbf{R}$. Thus all other eigenvalues of $\mathbf{R}$ are equal to ρ_2. In order to prove that $G \cong K_n$ we show that its diameter is one. For this reason, we show that G does not contain an induced shortest path P_m , $m \geq 3$.

Suppose that G contains an induced shortest path P_m , $m \geq 3$. Let $\mathbf{B}$ be the principal submatrix of $\mathbf{R}$ indexed by the vertices of P_m and let $\mu_i(\mathbf{B})$ denote the i-th eigenvalue of $\mathbf{B}$. Then by the interlacing theorem we obtain

$$\rho_i(\mathbf{R}) \geq \mu_i(\mathbf{B}) \geq \rho_{r-m+i}(\mathbf{R}) \quad , \quad i = 1, 2, \ldots, m$$

i. e.,

$$\rho_2 \geq \mu_2(\mathbf{B}) \geq \mu_3(\mathbf{B}) \geq \cdots \geq \rho_r = \rho_2 \ .$$

From this we conclude that P_m has at most two distinct Randić eigenvalues for $m \geq 3$, which is impossible. Therefore G does not contain two vertices at distance two or more, and hence it is complete graph. Conversely, if $G \cong K_n$, then all non-zero terms in $\mathbf{R}$ are equal to $1/(n-1)$ which implies that $\mathbf{R} = \frac{1}{n-1}\mathbf{A}$. Therefore $\rho_i = \frac{1}{n-1}\lambda_i$ for $i = 1, 2, \ldots, n$. From [1] it follows that G has exactly two distinct Randić eigenvalues 1 and $-1/(n-1)$. ■

4 Upper bound for Randić energy

In this section we present an upper bound for the Randić energy of graphs and characterize those graphs for which this bound is the best possible. Our considerations emulate those of Koolen and Moulton [31–33], used for estimating the ordinary graph energy.

Theorem 5. Let G be a simple connected graph. For any fixed values of $\alpha \in \mathbb{R}$ and $p \in \mathbb{N}$,

$$RE(G) \leq \sqrt{\frac{\sum_{i=1}^{n}\left(L_i^{(p+1)}\right)^2}{\sum_{i=1}^{n}\left(L_i^{(p)}\right)^2}} + \sqrt{(n-1)\left[2\sum_{i\sim j}\frac{1}{d_i\,d_j} - \frac{\sum_{i=1}^{n}\left(L_i^{(p+1)}\right)^2}{\sum_{i=1}^{n}\left(L_i^{(p)}\right)^2}\right]}. \tag{7}$$

Equality holds if and only if G is a complete graph or a connected graph satisfying

$$\frac{L_1^{(p+1)}}{L_1^{(p)}} = \frac{L_2^{(p+1)}}{L_2^{(p)}} = \cdots = \frac{L_n^{(p+1)}}{L_n^{(p)}} = k \geq \sqrt{\frac{2\sum_{i\sim j}\frac{1}{d_i\,d_j}}{n}}$$

with three distinct Randić eigenvalues

$$k \quad , \quad \sqrt{\frac{2\sum_{i\sim j}\frac{1}{d_i\,d_j} - k^2}{n-1}} \quad \text{and} \quad -\sqrt{\frac{2\sum_{i\sim j}\frac{1}{d_i\,d_j} - k^2}{n-1}}\ . \tag{8}$$

Proof. Let $\rho_1 \geq \rho_2 \geq \ldots \geq \rho_n$ be the Randić eigenvalues of G. We know that

$$\sum_{i=1}^{n}\rho_i = 0 \quad , \quad \sum_{i=1}^{n}|\rho_i| = RE(G) \quad , \quad \sum_{i=1}^{n}\rho_i^2 = 2\sum_{i\sim j}\frac{1}{d_i\,d_j}\ .$$

By the Cauchy–Schwarz inequality we get

$$\sum_{i=2}^{n}|\rho_i| \leq \sqrt{(n-1)\sum_{i=1}^{n}\rho_i^2} = \sqrt{(n-1)\left(2\sum_{i\sim j}\frac{1}{d_i\,d_j} - \rho_1^2\right)}. \tag{9}$$

Thus

$$RE(G) \leq \rho_1 + \sqrt{(n-1)\left(2\sum_{i\sim j}\frac{1}{d_i\,d_j} - \rho_1^2\right)}.$$

Again by the Cauchy–Schwarz inequality, we also get

$$R_i^2 = \left(\sum_{j=1}^{n}R_{ij}\right)^2 \leq n\sum_{j=1}^{n}R_{ij}^2\ .$$

Then

$$\sum_{i=1}^{n}R_i^2 \leq n\sum_{i=1}^{n}\sum_{j=1}^{n}R_{ij}^2 = 2n\sum_{i\sim j}\frac{1}{d_i\,d_j}\ .$$

Moreover

$$S_i = \sum_{j=1}^{n}R_{ij}R_j \geq \sum_{j=1}^{n}R_{ij}^2 \qquad \text{and} \qquad \sum_{i=1}^{n}S_i^2 \geq \sum_{i=1}^{n}\left(\sum_{j=1}^{n}R_{ij}^2\right)^2 \geq \left(2\sum_{i\sim j}\frac{1}{d_i\,d_j}\right)^2$$

resulting in

$$\rho_1 \geq \sqrt{\frac{\sum_{i=1}^{n} S_i^2}{\sum_{i=1}^{n} R_i^2}} \geq \sqrt{\frac{2}{n} \sum_{i \sim j} \frac{1}{d_i\, d_j}}\,. \tag{10}$$

By Theorem 4 and Eq. (10) we have

$$\rho_1 \geq \sqrt{\frac{\sum_{i=1}^{n} \left(L_i^{(p+1)}\right)^2}{\sum_{i=1}^{n} \left(L_i^{(p)}\right)^2}} \geq \sqrt{\frac{\sum_{i=1}^{n} S_i^2}{\sum_{i=1}^{n} R_i^2}} \geq \sqrt{\frac{2}{n} \sum_{i \sim j} \frac{1}{d_i\, d_j}}\,. \tag{11}$$

Let f be the function given by

$$f(x) = x + \sqrt{(n-1)\left(2 \sum_{i \sim j} \frac{1}{d_i\, d_j} - x^2\right)}$$

where $x \leq \sqrt{2 \sum_{i \sim j} 1/(d_i\, d_j)}$. By direct calculation it can be shown that f monotonically decreases for $x \geq \sqrt{(2/n) \sum_{i \sim j} 1/(d_i\, d_j)}$, from which it follows

$$RE(G) \leq f\left(\rho_1\right) \leq f\left(\sqrt{\frac{\sum_{i=1}^{n} \left(L_i^{(p+1)}\right)^2}{\sum_{i=1}^{n} \left(L_i^{(p)}\right)^2}}\right)$$

resulting in the inequality (7).

Now we suppose that the equality holds in (7). Then all inequalities in the above argument must be equalities. From (11) we have

$$\rho_1 = \sqrt{\frac{\sum_{i=1}^{n} \left(L_i^{(p+1)}\right)^2}{\sum_{i=1}^{n} \left(L_i^{(p)}\right)^2}}$$

which implies

$$\frac{L_1^{(p+1)}}{L_1^{(p)}} = \frac{L_2^{(p+1)}}{L_2^{(p)}} = \cdots = \frac{L_n^{(p+1)}}{L_n^{(p)}}\,.$$

In particular, by (9), we have

$$|\rho_i| = \sqrt{\frac{2 \sum_{i \sim j} \frac{1}{d_i\, d_j} - \rho_1^2(\mathbf{R})}{n-1}}$$

for $i = 2, \ldots, n$. Then there are three possibilities:

- G has only one distinct Randić eigenvalue. Since $\sum_{i=1}^{n} \rho_i = 0$ and G is connected, then $G \cong K_1$.

- G has exactly two distinct Randić eigenvalues. Then by Lemma 2, $G \cong K_n$ for some $n \geq 2$.

- G has exactly three distinct Randić eigenvalues. In this case,

$$\rho_1 = \sqrt{\frac{\sum_{i=1}^{n} \left(L_i^{(p+1)}\right)^2}{\sum_{i=1}^{n} \left(L_i^{(p)}\right)^2}} \qquad \text{and} \qquad |\rho_i| = \sqrt{\frac{2\sum_{i\sim j} \frac{1}{d_i\,d_j} - \rho_1^2}{n-1}}$$

for $i = 2, \ldots, n$. Since $L_i^{(p+1)}/L_i^{(p)} = k$ holds for all i, we get that G is a connected graph with three distinct Randić eigenvalues given by (8). Conversely, one can easily see that the equality in (7) holds for the graphs specified in the second part of the theorem. ■

By setting $\alpha = 1$ and $p = 1$ in (7), we obtain:

Corollary 2. Let G be a simple connected graph with Randić degree sequence $\{R_1, R_2, \ldots, R_n\}$ and second Randić degree sequence $\{S_1, S_2, \ldots, S_n\}$. Then

$$RE(G) \leq \sqrt{\frac{\sum_{i=1}^{n} S_i^2}{\sum_{i=1}^{n} R_i^2}} + \sqrt{(n-1)\left[2\sum_{i\sim j} \frac{1}{d_i\,d_j} - \frac{\sum_{i=1}^{n} S_i^2}{\sum_{i=1}^{n} R_i^2}\right]}. \tag{12}$$

Equality in (12) holds if and only if G is a complete graph or a pseudo k-Randić regular graph with three distinct Randić eigenvalues given by (8).

5 Concluding remarks

In this paper the Randić matrix and its eigenvalues, the Randić eigenvalues, are studied. Bounds obtained for the greatest Randić eigenvalue, referred to as the Randić spectral radius. A new bound for the Randić energy is also put forward. These bounds depend on the Randić degrees and the second

Randić degrees of the vertices, and become equalities when the underlying graph is Randić regular or pseudo Randić regular. We hope that this work will be accepted as a proper birthday present to Milan Randić, on the occasion of his 80-th anniversary.

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