

Randić Energy and Randić Eigenvalues*

Xueliang Li¹, Jianfeng Wang^{1,2,†}

¹Center for Combinatorics and LPMC-TJKLC, Nankai University,
Tianjin 300071, China

²Department of Mathematics, Qinghai Normal University, Xining,
Qinghai 810008, China

lxl@nankai.edu.cn, jfwang@aliyun.com

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Abstract

Let G be a graph of order n , and d_i the degree of a vertex v_i of G . The *Randić matrix* $\mathbf{R} = (r_{ij})$ of G is defined by $r_{ij} = 1/\sqrt{d_i d_j}$ if the vertices v_i and v_j are adjacent in G and $r_{ij} = 0$ otherwise. The *normalized signless Laplacian matrix* \mathcal{Q} is defined as $\mathcal{Q} = I + \mathbf{R}$, where I is the identity matrix. The *Randić energy* is the sum of absolute values of the eigenvalues of \mathbf{R} . In this paper, we find a relation between the normalized signless Laplacian eigenvalues of G and the Randić energy of its subdivision graph $S(G)$. We also give a necessary and sufficient condition for a graph to have exactly k and distinct Randić eigenvalues.

1 Introduction

All graphs considered here are simple, undirected and finite. Let G be a graph with vertex set $V(G) = \{v_1, v_2, \dots, v_n\}$ and degree sequence (d_1, d_2, \dots, d_n) , where d_i is the degree of a vertex v_i ($1 \leq i \leq n$) of G . For a graph G , let $M = M(G)$ be a corresponding *graph matrix* defined in a prescribed way. The *M -polynomial* of G is defined as $\phi_M(G, \lambda) = \det(\lambda I - M)$, where I is the identity matrix. The *M -eigenvalues* of G are those of its graph matrix M . It is well-known that there already exist some graph matrices, including *adjacency matrix* A , *degree matrix* D , *Laplacian matrix* $L = D - A$, *signless Laplacian matrix* $Q = D + A$ and so on.

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†Corresponding author.

In 1975, Milan Randić [17] invented a molecular structure descriptor defined as

$$R(G) = \sum_{i \sim j} \frac{1}{\sqrt{d_i d_j}},$$

where the summation goes over all pairs of adjacent vertices of the underlying (molecular) graph. This graph invariant is nowadays known under the name *Randić index*, for details see [10, 12, 13, 18].

Gutman et al. [11] pointed out that the Randić-index-concept is purposeful to produce a graph matrix of order n , named *Randić matrix* $\mathbf{R}(G)$, whose (i, j) -entry is defined as

$$r_{ij} = \begin{cases} \frac{1}{\sqrt{d_i d_j}} & \text{if } v_i \text{ and } v_j \text{ are adjacent vertices,} \\ 0 & \text{if the vertices } v_i \text{ and } v_j \text{ are not adjacent,} \\ 0 & \text{if } i = j. \end{cases}$$

In what follows, we need the convention that all graphs possess no isolated vertices. Then $\mathbf{R}(G) = D^{-\frac{1}{2}}AD^{-\frac{1}{2}}$. Recall that the *normalized Laplacian* and *signless Laplacian matrices* [5] are respectively defined as

$$\mathcal{L}(G) = D^{-\frac{1}{2}}LD^{-\frac{1}{2}} \quad \text{and} \quad \mathcal{Q}(G) = D^{-\frac{1}{2}}QD^{-\frac{1}{2}}.$$

From this point of view, the eigenvalues of above three matrices have a direct relation. As shown in [11], $\mathcal{L}(G) = I_n - \mathbf{R}(G)$ and $\mathcal{Q}(G) = I_n + \mathbf{R}(G)$. So if an \mathbf{R} -eigenvalue is ρ_i , then the \mathcal{L} -eigenvalue μ_i and \mathcal{Q} -eigenvalue θ_i are respectively

$$\mu_i = 1 - \rho_i \quad \text{and} \quad \theta_i = 1 + \rho_i, \quad 1 \leq i \leq n. \tag{1.1}$$

For the \mathcal{L} -eigenvalues, there are numerous results; see [5] for example. From Lemmas 1.7–1.8 [5] it follows that $0 \leq \mu_i \leq 2$, and so by (1.1),

$$-1 \leq \rho_i \leq 1 \quad \text{and} \quad 0 \leq \theta_i \leq 2, \quad 1 \leq i \leq n. \tag{1.2}$$

Gutman [9] introduced the (adjacency) energy of a graph G as follows

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

which has been extended to energies of other graph matrices [14, 16]. Especially, the *Randić energy* $RE(G)$ [1, 2] is defined as

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

So far, there are quite a few results about the Randić energy and \mathbf{R} -eigenvalues, which therefore becomes the main research objects of this paper. In the rest of the paper, we will give a relation between the \mathcal{Q} -eigenvalues of a graph and the Randić energy of its subdivision in Section 2. We also give a necessary and sufficient condition for a graph to have exactly k and distinct R -eigenvalues in Section 3, particularly for $k = 2, 3$.

2 Randić energy and \mathcal{Q} -eigenvalues

Let $S(G)$ be the subdivision of a graph G that is obtained by adding a new vertex into each edge of G . Evidently, $S(G)$ is a bipartite graph, and so $V(S(G)) = V_1 \cup V(G)$, where V_1 is the set of new added vertices of degree two.

The following lemma from matrix theory can be found in, for example, [6] p. 62.

Lemma 2.1 *If M is a nonsingular square matrix, then*

$$\begin{vmatrix} M & N \\ P & F \end{vmatrix} = |M| \cdot |F - PM^{-1}N|.$$

Lemma 2.2 *Let G be a graph with order n and size m . Then*

$$\phi_{\mathbf{R}}(S(G), \lambda) = \frac{\lambda^{m-n}}{2^n} \phi_{\mathcal{Q}}(G, 2\lambda^2).$$

Proof. Obviously, $|V(S(G))| = n + m$. It is well-known that

$$Q = BB^T \quad \text{and} \quad A(S(G)) = \begin{pmatrix} O & B^T \\ B & O \end{pmatrix},$$

where B is the incidence matrix of G and B^T is the transpose of B . Then, we partition the degree matrix $D(S(G))$ into

$$D(S(G)) = \begin{pmatrix} D_1^{-\frac{1}{2}} & O \\ O & D_2^{-\frac{1}{2}} \end{pmatrix},$$

where $D_1 = \text{diag}(2, 2, \dots, 2)$ with order $m \times m$ and $D_2 = D(G)$. If G has no isolated vertices, then so does $S(G)$. Consequently,

$$\begin{aligned} \mathbf{R}(S(G)) &= D^{-\frac{1}{2}} A(S(G)) D^{-\frac{1}{2}} = \begin{pmatrix} D_1^{-\frac{1}{2}} & O \\ O & D_2^{-\frac{1}{2}} \end{pmatrix} \begin{pmatrix} O & B^T \\ B & O \end{pmatrix} \begin{pmatrix} D_1^{-\frac{1}{2}} & O \\ O & D_2^{-\frac{1}{2}} \end{pmatrix} \\ &= \begin{pmatrix} O & D_1^{-\frac{1}{2}} B^T D_2^{-\frac{1}{2}} \\ D_2^{-\frac{1}{2}} B D_1^{-\frac{1}{2}} & O \end{pmatrix}. \end{aligned}$$

By Lemma 2.1 we get

$$\begin{aligned}
 \phi_{\mathbf{R}}(S(G), \lambda) &= |\lambda I_{m+n} - \mathbf{R}(S(G))| = \left| \begin{array}{cc} \lambda I_m & -D_1^{-\frac{1}{2}} B^T D_2^{-\frac{1}{2}} \\ -D_2^{-\frac{1}{2}} B^T D_1^{-\frac{1}{2}} & \lambda I_n \end{array} \right| \\
 &= |\lambda I_m| |\lambda I_n - D_2^{-\frac{1}{2}} B D_1^{-\frac{1}{2}} \frac{I_m}{\lambda} D_1^{-\frac{1}{2}} B^T D_2^{-\frac{1}{2}}| \\
 &= \lambda^{m-n} |\lambda^2 I_n - \frac{1}{2} D_2^{-\frac{1}{2}} B B^T D_2^{-\frac{1}{2}}| \\
 &= \frac{\lambda^{m-n}}{2^n} |2\lambda^2 I_n - \mathcal{Q}| \\
 &= \frac{\lambda^{m-n}}{2^n} \phi_{\mathcal{Q}}(G, 2\lambda^2).
 \end{aligned}$$

This finishes the proof.

Theorem 2.3 *Let G be a graph with order n and size m .*

- (i) *If $\phi_{\mathcal{Q}}(G, \lambda) = \sum_{i=0}^n a_i \lambda^{n-i}$, then $\phi_{\mathbf{R}}(S(G), \lambda) = \lambda^{m-n} \sum_{i=0}^n 2^{-i} a_i \lambda^{n-i}$.*
- (ii) *ρ is an \mathbf{R} -eigenvalue of $S(G)$ if and only if $2\rho^2$ is a \mathcal{Q} -eigenvalue of G .*
- (iii) *Let $\theta_1, \theta_2, \dots, \theta_n$ be the \mathcal{Q} -eigenvalues of G . Then $RE(S(G)) = \sqrt{2} \sum_{i=1}^n \sqrt{\theta_i}$.*

Proof. For (i), by Lemma 2.2 we get

$$\phi_{\mathbf{R}}(S(G), \lambda) = \frac{\lambda^{m-n}}{2^n} \phi_{\mathcal{Q}}(G, 2\lambda^2) = \frac{\lambda^{m-n}}{2^n} \sum_{i=0}^n a_i (\sqrt{2}\lambda)^{2(n-i)} = \lambda^{m-n} \sum_{i=0}^n 2^{-i} a_i \lambda^{n-i}.$$

(ii) is an immediate result of Lemma 2.2. For (iii), from (1.2) we obtain $\theta_i \geq 0$, and so $\pm\sqrt{\theta_i/2}$ is an \mathbf{R} -eigenvalue of $S(G)$ by (i). Thus, $RE(S(G)) = \sqrt{2} \sum_{i=1}^n \sqrt{\theta_i}$.

Lemma 2.4 *By Theorem 2.3(i), it becomes easier to compute the Randić energies of some graphs. As an example, Gutman et al. [11] conjectured that the connected graph with odd order and greatest Randić energy is the sun, which is exactly the subdivision of the star S_n . Easy to compute $\phi_{\mathcal{Q}}(S_n, \theta) = \theta(\theta-1)^{n-2}(\theta-2)$. Hence, $RE(S(S_n)) = \sqrt{2}n + 2 - 2\sqrt{2}$.*

3 Connected graphs with distinct \mathbf{R} -eigenvalues

A popular and important research field is to investigate the connected graphs with distinct eigenvalues. As van Dam said, it is an interplay between combinatorics and algebra; for details see his thesis [7]. Inspired by his ideas, we give a necessary and sufficient condition for a graph to have k distinct \mathbf{R} -eigenvalues.

It has been proved that $\rho_1 = 1$ is the largest \mathbf{R} -eigenvalues with the Perron-Frobenius vector $\alpha^T = (\sqrt{d_1}, \sqrt{d_2}, \dots, \sqrt{d_n})$; see [4, 11, 15].

Theorem 3.1 *Let G be connected graph with order $n \geq 3$ and size m . Then G has exactly k ($2 \leq k \leq n$) and distinct \mathbf{R} -eigenvalues if and only if there are $k - 1$ distinct none-one real numbers $\rho_2, \rho_3, \dots, \rho_k$ satisfying*

(i) $\mathbf{R} - \rho_i I$ is a singular matrix for $2 \leq i \leq k$;

(ii) $\prod_{i=2}^k (\mathbf{R} - \rho_i I) = \frac{\prod_{i=2}^k (1 - \rho_i)}{2m} \alpha \alpha^T$.

Moreover, $1, \rho_2, \dots, \rho_k$ are exactly the k distinct \mathbf{R} -eigenvalues of G .

Proof. Let $\rho_1 = 1, \rho_2, \rho_3, \dots, \rho_k$ be the k distinct \mathbf{R} -eigenvalues. Let α_i be the eigenvector belonging to ρ_i ($2 \leq i \leq k$). Then, $\mathbf{R}\alpha_i = \rho_i \alpha_i$, and so $(\mathbf{R} - \rho_i I)\alpha_i = 0$ which shows that 0 is an engenvalue of the matrix $\mathbf{R} - \rho_i I$ ($2 \leq i \leq k$). Hence, (i) follows. For (ii), since \mathbf{R} is a real symmetric matrix, it must be diagonalizable and thus the minimal polynomial of \mathbf{R} is $(\lambda - \rho_1)(\lambda - \rho_2) \cdots (\lambda - \rho_k)$. Hence,

$$\prod_{i=1}^k (\mathbf{R} - \rho_i I) = O, \quad \text{that is, } (\mathbf{R} - \rho_1 I)(\prod_{i=2}^k (\mathbf{R} - \rho_i I)) = O.$$

Since G is connected, by Perron-Frobenius Theorem we know that the algebraic multiplicity of $\rho_1 = 1$ is one, and so is the geometric multiplicity. Consequently, each column of $H = \prod_{i=2}^n (\mathbf{R} - \rho_i I) = (h_1, h_2, \dots, h_n)$ is a scalar multiple of the Perron-Frobenius vector α . Set $h_i = a_i \alpha$ ($1 \leq i \leq n$). So, $H = \alpha(a_1, a_2, \dots, a_n)$ and thus

$$\alpha^T H = \alpha^T \alpha (a_1, a_2, \dots, a_n).$$

By a direct calculation we have

$$\prod_{i=2}^k (1 - \rho_i) \alpha^T = 2m(a_1, a_2, \dots, a_n),$$

leading to

$$a_i = \frac{\prod_{i=2}^k (1 - \rho_i)}{2m} \sqrt{d_i} \quad (i = 1, 2, \dots, k).$$

The necessity thus follows.

For the sufficiency, from (i) it follows that the system of homogeneous linear equations $(\mathbf{R} - \rho_i I)\mathbf{x} = 0$ has non-zero solution, say α_i , and thus $\mathbf{R}\alpha_i = \rho_i \alpha_i$ which indicates that ρ_i is an eigenvalue of matrix \mathbf{R} ($2 \leq i \leq k$). Recall that $\rho_1 = 1$ is always an \mathbf{R} -eigenvalue. Therefore, we have shown that G has k distinct \mathbf{R} -eigenvalues $\rho_1 = 1, \rho_2, \dots, \rho_k$.

Assume that G has an extra \mathbf{R} -eigenvalue ρ_{k+1} . Set $f(x) = \prod_{i=2}^k (x - \rho_i)$. Easily to know $f(\rho_i)$ ($1 \leq i \leq k + 1$) is the eigenvalue of $f(\mathbf{R})$. Obviously, $f(\rho_1) \neq 0$, $f(\rho_i) = 0$

($2 \leq i \leq k$) and $f(\rho_{k+1}) \neq 0$. By (ii), the rank of $f(\mathbf{R})$ is one, and so $f(\mathbf{R})$ has only one none-zero simple eigenvalue, a contradiction.

Bozkurt et al. [2] determined the connected graphs with two distinct \mathbf{R} -eigenvalues. We now give another short proof based on the above theorem.

Corollary 3.2 *A connected graph G has exactly two and distinct \mathbf{R} -eigenvalues if and only if G is a complete graph with order at least two.*

Proof. It is known that the complete graph of order n has exactly two distinct \mathbf{R} -eigenvalues 1 and $-\frac{1}{n-1}$ [6]. Substituting $-\frac{1}{n-1}$ into Eq. (3.1) we get

$$\mathbf{R}(G) = \frac{n}{2m(n-1)}\alpha\alpha^T - \frac{1}{n-1}I.$$

Considering the diagonal entries in both sides of the above equality, we have

$$\frac{n}{2m(n-1)}d_i - \frac{1}{n-1} = 0,$$

and so $d_i = \frac{2m}{n}$ ($i = 1, 2, \dots, n$), i.e., G is a regular graph. Comparing the non-diagonal entries in both sides of the above equality we get $r_{ij} = \frac{1}{n-1}$ ($i \neq j$) and thus G is the complete graph.

For the graph with exactly three and distinct \mathbf{R} -eigenvalues, the following characterization is given. We denote the number of common neighbors by δ_{ij} if vertices v_i and v_j are adjacent, and by σ_{ij} if they are not.

Corollary 3.3 *Let $c = \frac{\prod_{i=2}^k(1-\rho_i)}{2m}$. A connected graph G has exactly three and distinct \mathbf{R} -eigenvalues $1, \rho_2, \rho_3$ if and only if the following items hold:*

- (i) *for any vertex u_i , $\sum_{v_j \sim u_i} \frac{1}{d_j} = cd_i^2 - \rho_2\rho_3d_i$,*
- (ii) *for adjacent vertices u_i and v_j , $\delta_{ij} = cd_id_j + \rho_2 + \rho_3$,*
- (iii) *for nonadjacent vertices u_i and v_j , $\sigma_{ij} = cd_id_j$.*

Proof. From Theorem 3.1 we get $(\mathbf{R} - \rho_2I)(\mathbf{R} - \rho_3I) = c\alpha\alpha^T$. Then the results follow by considering the diagonal entries and nondiagonal entries for both sides of this equality.

Note that a k -regular graph of order n ($0 < k < n-1$) is *strong regular* with parameters (n, k, δ, σ) if the number of common neighbors of any two distinct vertices equals δ if the vertices are adjacent and σ otherwise [3]. The following result follows from Corollary 3.3.

Corollary 3.4 *A regular connected graph has exactly three and distinct \mathbf{R} -eigenvalues if and only if it is strong regular.*

From (1.1) it follows that a connected graph has exactly k distinct \mathbf{R} -eigenvalues if and only if it has k distinct \mathcal{L} -ones. van Dam and Omidi [8] found such graphs and pointed out that a complete classification of such graphs still seems out of reach. In subsequent work, it seems interesting to determine connected graphs with exactly four or more and distinct \mathbf{R} -eigenvalues. Furthermore, due to $\mathcal{L} = I - \mathbf{R}$, it seems much simpler to investigate on this topic by the \mathbf{R} -eigenvalues.

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