Randić Energy and Randić Eigenvalues*

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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 $V(G) = \{v_1, v_2, \cdots, v_n\}$ and degree sequence $(d_1, d_2, \cdots, d_n)$, 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.

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

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

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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

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

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

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

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

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

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),

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

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 $D_1 = \text{diag}(2, 2, \cdots, 2)$ 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

$$\begin{aligned}\phi_{\mathbf{R}}(S(G),\lambda) = |\lambda I_{m+n} - \mathbf{R}(S(G))| &= \begin{vmatrix} \lambda I_m & -D_1^{-\frac{1}{2}}B^T D_2^{-\frac{1}{2}} \\ -D_2^{-\frac{1}{2}}B^T D_1^{-\frac{1}{2}} & \lambda I_n \end{vmatrix} \\ &= |\lambda I_m||\lambda I_n - D_2^{-\frac{1}{2}}BD_1^{-\frac{1}{2}}\frac{I_m}{\lambda}D_1^{-\frac{1}{2}}B^T D_2^{-\frac{1}{2}}| \\ &= \lambda^{m-n}|\lambda^2 I_n - \frac{1}{2}D_2^{-\frac{1}{2}}BB^T D_2^{-\frac{1}{2}}| \\ &= \frac{\lambda^{m-n}}{2^n}|2\lambda^2 I_n - \mathcal{Q}| \\ &= \frac{\lambda^{m-n}}{2^n}\phi_{\mathcal{Q}}(G,2\lambda^2).\end{aligned}$$

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 $\theta_1, \theta_2, \cdots, \theta_n$ 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 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 $\alpha^T = (\sqrt{d_1}, \sqrt{d_2}, \cdots, \sqrt{d_n})$; 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 $\rho_2, \rho_3, \cdots, \rho_k$ satisfying*

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

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

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

Proof. Let $\rho_1 = 1, \rho_2, \rho_3, \cdots, p_k$ 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,

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

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 $H = \Pi_{i=2}^{n}(\mathbf{R} - \rho_i I) = (h_1, h_2, \cdots, h_n)$ is a scalar multiple of the Perron-Frobenius vector α. Set $h_i = a_i\alpha$ $(1 \leq i \leq n)$. So, $H = \alpha(a_1, a_2, \cdots, a_n)$ and thus

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

By a direct calculation we have

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

leading to

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

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 $\mathbf{R}$ $(2 \le i \le k)$. Recall that $\rho_1 = 1$ is always an $\mathbf{R}$-eigenvalue. Therefore, we have shown that G has k distinct $\mathbf{R}$-eigenvalues $\rho_1 = 1, \rho_2, \cdots, \rho_k$.

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 $f(\rho_i)$ $(1 \le i \le k+1)$ is the eigenvalue of $f(\mathbf{R})$. Obviously, $f(\rho_1) \neq 0$, $f(\rho_i) = 0$ $(2 \le i \le k)$ 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 $d_i = \frac{2m}{n}$ $(i = 1, 2, \cdots, n)$, 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, $\sum_{v_j \sim u_i} \frac{1}{d_j} = cd_i^2 - \rho_2 \rho_3 d_i$,

(ii) *for adjacent vertices* u_i *and* v_j, $\delta_{ij} = cd_i d_j + \rho_2 + \rho_3$,

(iii) *for nonadjacent vertices* u_i *and* v_j, $\sigma_{ij} = cd_i d_j$.

Proof. From Theorem 3.1 we get $(\mathbf{R} - \rho_2 I)(\mathbf{R} - \rho_3 I) = c\alpha\alpha^T$. 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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