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 \(R = (r_{ij})\) of \(G\) is defined by \(r_{ij} = 1/\sqrt{d_j d_j}\) if the vertices \(v_i\) and \(v_j\) are adjacent in \(G\) and \(r_{ij} = 0\) otherwise. The normalized signless Laplacian matrix \(Q\) is defined as \(Q = I + R\), where \(I\) is the identity matrix. The Randić energy is the sum of absolute values of the eigenvalues of \(R\).

In this paper, we find a relation between the normalized signless Laplacian eigenvalues of \(G\) and the Randić energy of its subdivided 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 \(V(G) = \{v_1, v_2, \ldots, v_n\}\) and degree sequence \((d_1, d_2, \ldots, d_n)\), 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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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 \( R(G) \), 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 \( R(G) = D^{-\frac{1}{2}}A D^{-\frac{1}{2}} \). Recall that the normalized Laplacien and sinless Laplacian matrices \([5]\) are respectively defined as

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

From this point of view, the eigenvalues of above three matrices have a direct relation. As shown in [11], \( L(G) = I_n - R(G) \) and \( Q(G) = I_n + R(G) \). So if an \( R \)-eigenvalue is \( \rho_i \), then the \( L \)-eigenvalue \( \mu_i \) and \( Q \)-eigenvalue \( \theta_i \) are respectively

\[
 \mu_i = 1 - \rho_i \quad \text{and} \quad \theta_i = 1 + \rho_i, \quad 1 \leq i \leq n.
\]

For the \( L \)-eigenvalues, there are numerous results; see [5] for example. From Lemmas 1.7–1.8 \([4]\) it follows that \( 0 \leq \mu_i \leq 2 \), and so by (1),

\[
 -1 \leq \rho_i \leq 1 \quad \text{and} \quad 0 \leq \theta_i \leq 2, \quad 1 \leq i \leq n.
\]

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 \([14] [10]\). 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 \( R \)-eigenvalues, which therefore becomes the main research objects of this paper. In the rest of the paper, we will give a relation between the \( Q \)-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

\[
\phi_R(S(G), \lambda) = \frac{\lambda^{m-n}}{2n} \phi_Q(G, 2\lambda^2).
\]

**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 incident 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,

\[
R(S(G)) = D^{-\frac{1}{2}}A(S(G))D^{-\frac{1}{2}} = \begin{pmatrix} D_1^{-\frac{1}{2}} & O \\ O & D_2^{-\frac{1}{2}} \end{pmatrix} \begin{pmatrix} O & B^T \\ B & O \end{pmatrix} \begin{pmatrix} D_1^{-\frac{1}{2}} & O \\ O & D_2^{-\frac{1}{2}} \end{pmatrix} = \begin{pmatrix} O & D_1^{-\frac{1}{2}}B^TD_2^{-\frac{1}{2}} \\ D_2^{-\frac{1}{2}}BD_1^{-\frac{1}{2}} & O \end{pmatrix}.
\]

By Lemma 2.1 we get

\[
\phi_R(S(G), \lambda) = |\lambda I_{m+n} - R(S(G))| = \begin{vmatrix} \lambda I_m & -D_1^{-\frac{1}{2}}B^TD_2^{-\frac{1}{2}} \\ -D_2^{-\frac{1}{2}}B^TD_1^{-\frac{1}{2}} & \lambda I_n \end{vmatrix}
\]

\[
= |\lambda I_m| |\lambda I_n - D_2^{-\frac{1}{2}}BD_1^{-\frac{1}{2}}I_m D_1^{-\frac{1}{2}}B^TD_2^{-\frac{1}{2}}| 
\]

\[
= \lambda^{m-n} |\lambda^2 I_n - \frac{1}{2}D_2^{-\frac{1}{2}}BBD_2^{-\frac{1}{2}}| 
\]

\[
= \frac{\lambda^{m-n}}{2n} |2\lambda^2 I_n - \mathcal{Q}| 
\]

\[
= \frac{\lambda^{m-n}}{2n} \phi_Q(G, 2\lambda^2).
\]

This finishes the proof. \( \square \)
Theorem 3.1. Let \( G \) be a graph with order \( n \) and size \( m \).

(i) If \( \phi_Q(G, \lambda) = \sum_{i=0}^{n} a_i \lambda^{n-i} \), then \( \phi_R(G, \lambda) = \lambda^{m-n} \sum_{i=0}^{n} 2^{-i} a_i \lambda^{n-i} \).

(ii) \( \rho \) is an \( R \)-eigenvalue of \( G \) if and only if \( 2\rho^2 \) is a \( Q \)-eigenvalue of \( G \).

(iii) Let \( \theta_1, \theta_2, \cdots, \theta_n \) be the \( Q \)-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

\[
\phi_R(G, \lambda) = \frac{\lambda^{m-n}}{2^n} \phi_Q(G, 2\lambda^2) = \frac{\lambda^{m-n}}{2^n} \sum_{i=0}^{n} a_i (\sqrt{2}\lambda)^{2(n-i)} = \lambda^{m-n} \sum_{i=0}^{n} 2^{-i} a_i \lambda^{n-i}.
\]

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

Remark 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 \( \phi_Q(S_n, \theta) = \theta(\theta - 1)^{n-2}(\theta - 2) \). Hence, \( RE(S(S_n)) = \sqrt{2n + 2 - 2\sqrt{2}} \).

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 \( R \)-eigenvalues.

It has been proved that \( \rho_1 = 1 \) is the largest \( R \)-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 \( R \)-eigenvalues if and only if there are \( k-1 \) distinct none-one real numbers \( \rho_2, \rho_3, \cdots, \rho_k \) satisfying

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

Moreover, \( 1, \rho_2, \cdots, \rho_k \) are exactly the \( k \) distinct \( R \)-eigenvalues of \( G \).

Proof. Let \( \rho_1 = 1, \rho_2, \rho_3, \cdots, \rho_k \) be the \( k \) distinct \( R \)-eigenvalues. Since \( R \) is a real symmetric matrix, it must be diagonalizable, and thus the minimal polynomial of \( R \) is \( (\lambda - \rho_1)(\lambda - \rho_2)\cdots(\lambda - \rho_k) \). Hence,

\[
\prod_{i=1}^{n} (R - \rho_i I) = O, \quad \text{that is,} \quad (R - \rho_1 I)(\prod_{i=2}^{n} (R - \rho_i I)) = O.
\]
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 $H = \prod_{i=2}^{n}(R - \rho_i I) = (h_1, h_2, \cdots, h_n)$ is a scalar multiple of the Perron-Frobenius vector $\alpha$. 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, multiplying $R - \rho_1 I$ ($\rho_1 = 1$) to both sides of (3), we arrive at

$$(R - \rho_1 I) \prod_{i=2}^{k}(R - \rho_i I) = \prod_{i=2}^{k}(1 - \rho_i) \alpha^T((R - I) \alpha) = O.$$ 

So, $m(x) = (x - \rho_1)(x - \rho_2) \cdots (x - \rho_k)$ is an annihilating polynomial of $R$, i.e., a polynomial with value at $R$ is a 0-matrix. From (3) follows $\prod_{i=2}^{k}(R - \rho_i I) \neq O$, which shows that the product of some factors taken from \{x - \rho_2, \cdots, x - \rho_k\} is not a minimal polynomial of $R$. Hence, $m(x)$ is the minimal polynomial, and thus $1, \rho_2, \cdots, \rho_k$ are the $k$ distinct $R$-eigenvalues.

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

**Corollary 3.2.** A connected graph $G$ has exactly two and distinct $R$-eigenvalues if and only if $G$ is a complete graph.

**Proof.** It is known that the complete graph of order $n$ has exactly two distinct $R$-eigenvalues $1$ and $-\frac{1}{n-1}$ [3]. Substituting $1$ and $-\frac{1}{n-1}$ into Eq. (3) we get

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

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

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

and so $d_i = n - 1$ ($i = 1, 2, \cdots, n$). Hence, $G$ is a complete graph. 

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

**Corollary 3.3.** Let $c = \prod_{i=2}^{k} (1 - \rho_i)$. A connected graph $G$ has exactly three and distinct $R$-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 $(R - \rho_2 I)(R - \rho_3 I) = c\alpha\alpha^T$. 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 $(n, k, \delta, \sigma)$ if the number of common neighbors of any two distinct vertices equals $\delta$ if the vertices are adjacent and $\sigma$ otherwise [3]. The following result follows from Corollary 3.3.

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

From (1) it follows that a connected graph has exactly $k$ distinct $R$-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 $R$-eigenvalues. Furthermore, due to $\mathcal{L} = I - R$, it seems much simpler to investigate on this topic by the $R$-eigenvalues.

**References**

[1] Ş.B. Bozkurt, A.D. Güngör, I. Gutman, A.S. Çevik, Randić matrix and Randić energy, MATCH Commun. Math. Comput. Chem. 64 (2010) 239–250.

[2] Ş.B. Bozkurt, A.D. Güngör, I. Gutman, Randić spectral radius and Randić energy, MATCH Commun. Math. Comput. Chem. 64 (2010) 321–334.

[3] A.E. Brouwer, W.H. Haemers, Spectra of graphs, [http://homepages.cwi.nl/~aeb/math/ipm.pdf](http://homepages.cwi.nl/~aeb/math/ipm.pdf) (October 2010).

[4] M. Cavers, S. Fallat, S. Kirkland, On the normalized Laplacian energy and general Randić index $R_1$ of graphs, Linear Algebra Appl. 433 (2010) 172–190.
[5] F.R.K. Chung, Spectral Graph Theory, Amer. Math. Soc., Providence, 1997.

[6] D.M. Cvetković, M. Doob, H. Sachs, Spectra of Graphs - Theory and Applications, Academic Press, New York, San Francisco, London, 1980.

[7] E.R. van Dam, Graphs with few eigenvalues: An interplay between combinatorics and algebra, PhD Thesis, Tilburg University, 1996.

[8] E.R. van Dam, G.R. Omidi, Graphs whose normalized Laplacian has three eigenvalues, Linear Algebra Appl. 435 (2011) 2560–2569.

[9] I. Gutman, The energy of a graph, Ber. Math. Statist. Sekt. Forschungsz. Graz, 103(1978), 1–22.

[10] I. Gutman, B. Furtula (Eds.), Recent Results in the Theory of Randić Index, Univ. Kragujevac, Kragujevac, 2008.

[11] I. Gutman, B. Furtula, S.B. Bozkurt, On Randić energy, Linear Algebra Appl. 442 (2014) 50–57.

[12] X. Li, I. Gutman, Mathematical Aspects of Randić-Type Molecular Structure Descriptors, Univ. Kragujevac, Kragujevac, 2006.

[13] X. Li, Y. Shi, A survey on the Randić index, MATCH Commun. Math. Comput. Chem. 59 (2008) 127–156.

[14] X. Li, Y. Shi, I. Gutman, Graph Energy, Springer, New York, 2012.

[15] B. Liu, Y. Huang, J. Feng, A note on the Randić spectral radius, MATCH Commun. Math. Comput. Chem. 68 (2012) 913–916.

[16] V. Nikiforov, The energy of graphs and matrices, J. Math. Anal. Appl. 326 (2007) 1472–1475.

[17] M. Randić, On characterization of molecular branching, J. Amer. Chem. Soc. 97 (1975) 6609–6615.

[18] M. Randić, On history of the Randić index and emerging hostility toward chemical graph theory, MATCH Commun. Math. Comput. Chem. 59 (2008) 5–124.