Randić Matrix and Randić Energy

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Abstract

If G is a graph on n vertices, and d_i is the degree of its i-th vertex, then 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. This matrix in a natural way occurs within Laplacian spectral theory, and provides the non-trivial part of the so-called normalized Laplacian matrix. In spite of its obvious relation to the famous Randić index, the Randić matrix seems to have not been much studied in mathematical chemistry. In this paper, we define the *Randić energy* as the sum of the absolute values of the eigenvalues of the Randić matrix, and establish some of its properties, in particular lower and upper bounds for it.

1 Introduction: Randić matrix

Let G be a simple graph and let $v_1, v_2, \ldots, v_n$ be its vertices. For $i = 1, 2, \ldots, n$, by d_i we denote the degree (the number of first neighbors) of the vertex v_i. Then the molecular structure–descriptor, put forward in 1975 by Milan Randić [1], is defined as

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

where $\sum\limits_{i \sim j}$ indicates summation over all pairs of adjacent vertices v_i, v_j. Nowadays, R is referred to as the *Randić index*.

The Randić index found countless chemical applications and became a popular topic of research in mathematics and mathematical chemistry [2–7].

The summands on the right–hand side of formula (1) may be understood as matrix elements. This observation may serve as a motivation for conceiving a symmetric square matrix $\mathbf{R} = \mathbf{R}(G) = \|R_{ij}\|$ of order n, defined via

$$R_{ij} = \begin{cases} 0 & \text{if } i = j \\ \dfrac{1}{\sqrt{d_i\, d_j}} & \text{if the vertices } v_i \text{ and } v_j \text{ of } G \text{ are adjacent} \\ 0 & \text{if the vertices } v_i \text{ and } v_j \text{ of } G \text{ are not adjacent.} \end{cases} \tag{2}$$

We propose that $\mathbf{R}$ be called the *Randić matrix* (of the graph G).

At this point it is purposeful to recall the definition of the adjacency matrix $\mathbf{A}$ of the graph G. Its (i, j)-entry is defined as:

$$A_{ij} = \begin{cases} 0 & \text{if } i = j \\ 1 & \text{if the vertices } v_i \text{ and } v_j \text{ of } G \text{ are adjacent} \\ 0 & \text{if the vertices } v_i \text{ and } v_j \text{ of } G \text{ are not adjacent.} \end{cases}$$

The connection between the Randić matrix and the Randić index is obvious: The sum of all elements of $\mathbf{R}$ is equal to $2R$. It is interesting that in spite of the enormous number of researches on (mathematical properties of) Randić index [4,6,7], its matrix counterpart has not been much used. To our best knowledge, only a few papers [8–11] employ Randić–matrix arguments in the study of Randić index. The works [8,9] present bounds for R in terms of the eigenvalues of the normalized Laplacian matrix (see below). The papers [10] and [11] explicitly use the matrix $\mathbf{R}$, calling it "*weighted adjacency matrix*" [10] and "*degree–adjacency matrix*" [11].

In Section 3 of this paper we will see that the Randić matrix plays an outstanding role in the theory of Laplacian graph spectra.

2 Introduction: Energies

Graph spectral theory, based on the eigenvalues of the adjacency matrix, has well and long known applications in chemistry [12–17]. One of the chemically (and also mathematically) most interesting graph–spectrum–based quantities is the graph energy, defined as follows.

Let G be a simple graph on n vertices, and let $\mathbf{A}$ be its adjacency matrix. Let $\lambda_1, \lambda_2, \ldots, \lambda_n$ be the eigenvalues of $\mathbf{A}$. These are said to be the eigenvalues of the graph G and to form its spectrum [13]. The *energy* $E(G)$ of the graph G is defined as the sum of the absolute values of its eigenvalues

$$E = E(G) = \sum_{i=1}^{n} |\lambda_i| \ . \tag{3}$$

For details on graph energy see the reviews [18–21], the papers published in this issue of *MATCH*, and the references cited therein.

In view of the evident success of the concept of graph energy, and because of the rapid decrease of open mathematical problems in its theory, energies based of the eigenvalues of other graph matrices have, one–by–one, been introduced. Of these, the *Laplacian energy* $LE(G)$, pertaining to the Laplacian matrix, seems to be the first [22,23]. Followed the *distance energy* [24,25], based on the distance matrix, and a variety of energy–like graph invariants introduced by Consonni and Todeschini [26]. Nikiforov extended the definition of energy to arbitrary matrices [27], making thus possible to conceive the *incidence energy* [28,29], based on the incidence matrix, etc. etc.

Along these lines of reasoning, we could think of the *Randić energy*, as the sum of absolute values of the eigenvalues of the Randić matrix. More formally: Let $\rho_1, \rho_2, \ldots, \rho_n$ be the eigenvalues of the Randić matrix $\mathbf{R}(G)$. Knowing that these eigenvalues are necessarily real numbers, and that their sum is zero, the Randić energy can be defined as

$$RE = RE(G) = \sum_{i=1}^{n} |\rho_i| \ . \tag{4}$$

This definition is applicable to all graphs.

Yet, the actual route to Randić energy is somewhat less straightforward.

3 The Laplacian spectral connection

For the considerations in this paper important is the Laplacian matrix and the energies associated with it.

The theory of Laplacian spectra is nowadays a well developed part of algebraic graph theory. Its details can be found in the reviews [20–25] and monographs [6,26].

Let $\mathbf{D}$ be the diagonal matrix of order n whose i-th diagonal entry is d_i, the degree of the vertex v_i of the graph G. Then the Laplacian matrix of G is defined as $\mathbf{L} = \mathbf{D} - \mathbf{A}$. Its eigenvalues $\mu_1, \mu_2, \ldots, \mu_n$ form the Laplacian spectrum of G.

In view of the fact that the Laplacian eigenvalues are non-negative real numbers, and that their sum is equal to $2m$, where m is the number of edges of G, the Laplacian analogue of Eq. (3), namely the Laplacian energy had to be defined as [22]

$$LE = LE(G) = \sum_{i=1}^{n} \left| \mu_i - \frac{2m}{n} \right| .$$

The term $2m/n$ has to be subtracted from the Laplacian eigenvalues, because then

$$\sum_{i=1}^{n} \left(\mu_i - \frac{2m}{n} \right) = 0 .$$

In the mathematical literature, also another form of the Laplacian matrix has been considered, named "normalized Laplacian matrix" (see, for instance [17, pp. 212–216]). Note, however, that in the book [36] this matrix is called "Laplacian matrix", which may cause quite some confusion. The latter terminology was used also by Araujo and de la Peña [8,9].

If $d_i = 0$ then the corresponding vertex v_i is said to be isolated. Suppose that the graph G has no isolated vertices. Then the matrix $\mathbf{D}^{-1/2}$ exists.[1] For a graph without isolated vertices, the *normalized Laplacian matrix* is defined as [17,36]

$$\tilde{\mathbf{L}} = \mathbf{D}^{-1/2}\,\mathbf{L}\,\mathbf{D}^{-1/2}$$

from which immediately follows that

$$\tilde{\mathbf{L}} = \mathbf{I} - \mathbf{D}^{-1/2}\,\mathbf{A}\,\mathbf{D}^{-1/2}$$

[1]Recall that $\mathbf{D}^{-1/2}$ is the diagonal matrix whose i-th diagonal entry is $1/\sqrt{d_i}$.

where $\mathbf{I}$ is the unit matrix of order n.

By direct matrix multiplication it can now be verified that

$$\mathbf{D}^{-1/2}\,\mathbf{A}\,\mathbf{D}^{-1/2} = \mathbf{R}\ .$$

Although elementary, the following result deserves to be stated as:

Theorem 1. *Let G be a graph without isolated vertices. Its normalized Laplacian matrix and Randić matrix are related as*

$$\tilde{\mathbf{L}} = \mathbf{I} - \mathbf{R}\ . \tag{5}$$

At this point it is worth noting that, in contrast to the normalized Laplacian matrix, the Randić matrix is well defined for all graphs, namely also for graphs possessing isolated vertices.

In analogy to other graph energies, we could now define the *normalized Laplacian energy*. Let $\tilde{\mu}_1, \tilde{\mu}_2, \ldots, \tilde{\mu}_n$ be the eigenvalues of $\tilde{\mathbf{L}}$. In view of the fact that these normalized Laplacian eigenvalues are non-negative real numbers, and that their sum is equal to n, the normalized Laplacian energy would be

$$NLE = NLE(G) = \sum_{i=1}^{n} |\tilde{\mu}_i - 1|\ . \tag{6}$$

The term $n/n = 1$ has to be subtracted from the normalized Laplacian eigenvalues, because then

$$\sum_{i=1}^{n} (\tilde{\mu}_i - 1) = 0\ .$$

However, there is no need introduce this new kind of Laplacian energy. Namely, we have:

Theorem 2. *If G is a graph without isolated vertices, then the quantity $NLE(G)$, defined via Eq. (6), coincides with the Randić energy $RE(G)$, defined via Eq. (4).*

Proof. Because of Eq. (5), $\tilde{\mu}_i = 1 - \rho_i$ for $i = 1, 2, \ldots, n$. Therefore

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

4 Bounds for Randić energy

In this section we first calculate $tr(\mathbf{R}^2)$, $tr(\mathbf{R}^3)$, and $tr(\mathbf{R}^4)$, where tr denotes the trace of a matrix. Moreover, using these equalities we obtain an upper and a lower bound for Randić energy of the graph G.

In order to obtain our main results we give the following:

Lemma 3. *Let G be a graph with n vertices and Randić matrix $\mathbf{R}$. Then*

$$
\begin{aligned}
tr(\mathbf{R}) &= 0 \\
tr(\mathbf{R}^2) &= 2\sum_{i\sim j}\frac{1}{d_i\,d_j} \\
tr(\mathbf{R}^3) &= 2\sum_{i\sim j}\frac{1}{d_i\,d_j}\left(\sum_{k\sim i\,,\,k\sim j}\frac{1}{d_k}\right) \\
tr(\mathbf{R}^4) &= \sum_{i=1}^{n}\left(\sum_{i\sim j}\frac{1}{d_i\,d_j}\right)^2+\sum_{i\neq j}\frac{1}{d_i\,d_j}\left(\sum_{k\sim i\,,\,k\sim j}\frac{1}{d_k}\right)^2 .
\end{aligned}
$$

Proof. By definition, the diagonal elements of $\mathbf{R}$ are equal to zero. Therefore the trace of $\mathbf{R}$ is zero.

Next, we calculate the matrix $\mathbf{R}^2$. For $i=j$

$$(\mathbf{R}^2)_{ii}=\sum_{j=1}^{n}R_{ij}\,R_{ji}=\sum_{j=1}^{n}(R_{ij})^2=\sum_{i\sim j}(R_{ij})^2=\sum_{i\sim j}\frac{1}{d_i\,d_j}$$

whereas for $i\neq j$

$$(\mathbf{R}^2)_{ij}=\sum_{k=1}^{n}R_{ik}\,R_{kj}=R_{ii}\,R_{ij}+R_{ij}\,R_{jj}+\sum_{k\sim i\,,\,k\sim j}R_{ik}\,R_{kj}=\frac{1}{\sqrt{d_i\,d_j}}\sum_{k\sim i\,,\,k\sim j}\frac{1}{d_k} .$$

Therefore

$$tr(\mathbf{R}^2)=\sum_{i=1}^{n}\sum_{i\sim j}\frac{1}{d_i\,d_j}=2\sum_{i\sim j}\frac{1}{d_i\,d_j} .$$

Since the diagonal elements of $\mathbf{R}^3$ are

$$(\mathbf{R}^3)_{ii}=\sum_{j=1}^{n}R_{ij}\,(\mathbf{R}^2)_{jk}=\sum_{i\sim j}\frac{1}{\sqrt{d_i\,d_j}}\,(\mathbf{R}^2)_{ij}=\sum_{i\sim j}\frac{1}{d_i\,d_j}\left(\sum_{k\sim i\,,\,k\sim j}\frac{1}{d_k}\right)$$

we obtain

$$tr(\mathbf{R}^3) = \sum_{i=1}^{n} \sum_{i \sim j} \frac{1}{d_i\, d_j} \left(\sum_{k \sim i\,,\, k \sim j} \frac{1}{d_k} \right) = 2 \sum_{i \sim j} \frac{1}{d_i\, d_j} \left(\sum_{k \sim i\,,\, k \sim j} \frac{1}{d_k} \right) .$$

We now calculate $tr(\mathbf{R}^4)$. Because $tr(\mathbf{R}^4) = \|\mathbf{R}^2\|_F^2$, where $\|\mathbf{R}^2\|_F$ denotes the Frobenius norm of $\mathbf{R}^2$, we obtain

$$\begin{aligned} tr(\mathbf{R}^4) &= \sum_{i,j=1}^{n} \left|(\mathbf{R}^2)_{ij}\right|^2 = \sum_{i=j} \left|(\mathbf{R}^2)_{ij}\right|^2 + \sum_{i \neq j} \left|(\mathbf{R}^2)_{ij}\right|^2 \\ &= \sum_{i=1}^{n} \left(\sum_{i \sim j} \frac{1}{d_i\, d_j} \right)^2 + \sum_{i \neq j} \frac{1}{d_i\, d_j} \left(\sum_{k \sim i\,,\, k \sim j} \frac{1}{d_k} \right)^2 . \end{aligned}$$

By this the proof of Lemma 3 is completed. ■

We mention in passing that the expression $\sum\limits_{i \sim j} 1/(d_i\, d_j)$, equal to the half of $tr(\mathbf{R}^2)$, is just a special case of the general Randić index $R_\alpha = \sum\limits_{i \sim j} (d_i\, d_j)^\alpha$ for $\alpha = -1$; for details see [4]. The very same quantity was considered by Miličević et al. [37] under the name “modified second Zagreb index”.

Theorem 4. *Let G be a graph with n vertices. Then*

$$RE \leq \sqrt{2n \sum_{i \sim j} \frac{1}{d_i\, d_j}} \,. \tag{7}$$

Equality in (7) is attained if and only if G is the graph without edges, or if all its vertices have degree one.

Proof. The variance of the numbers $|\rho_i|$, $i = 1, 2, \ldots, n$, is equal to

$$\frac{1}{n} \sum_{i=1}^{n} |\rho_i|^2 - \left(\frac{1}{n} \sum_{i=1}^{n} |\rho_i| \right)$$

and is greater than or equal to zero. Now,

$$\sum_{i=1}^{n} |\rho_i|^2 = \sum_{i=1}^{n} \rho_i^2 = tr(\mathbf{R}^2)$$

and therefore

$$\frac{1}{n}\, tr(\mathbf{R}^2) - \left(\frac{1}{n}\, RE \right)^2 \geq 0 \qquad \Longleftrightarrow \qquad RE \leq \sqrt{n\, tr(\mathbf{R}^2)} \,.$$

Inequality (7) follows from Lemma 3.

If G has no edges, then $\rho_i = 0$ for all $i = 1, 2, \ldots, n$, and therefore $RE = 0$ (cf. Theorem 6). Since there are no adjacent vertices, $\sum\limits_{i \sim j} 1/(d_i\, d_j)$ is also equal to zero. If G is a regular graph of degree one, then $\rho_i = \pm 1$ (cf. Theorem 6), implying that the variance of $|\rho_i|$, $i = 1, 2, \ldots, n$, is zero. This implies equality in (7).

For all other graphs the eigenvalues of $\mathbf{R}(G)$ are not all equal by absolute value. Therefore, the variance of of $|\rho_i|$, $i = 1, 2, \ldots, n$, is greater than zero, implying that the inequality (7) is strict. ■

It should be noted that Theorem 4 is just the Randić–energy variant of the classical McClelland inequality [18–20].

Theorem 5. *Let G be a graph with n vertices and at least one edge. Then*

$$RE(G) \geq 2 \sum_{i \sim j} \frac{1}{d_i\, d_j} \sqrt{\frac{2 \sum\limits_{i \sim j} \frac{1}{d_i\, d_j}}{\sum\limits_{i=1}^{n} \left(\sum\limits_{i \sim j} \frac{1}{d_i\, d_j} \right)^2 + \sum\limits_{i \neq j} \frac{1}{d_i\, d_j} \left(\sum\limits_{k \sim i\,,\, k \sim j} \frac{1}{d_k} \right)^2}}\ .$$

Proof. Our starting point is the Hölder inequality

$$\sum_{i=1}^{n} a_i\, b_i \leq \left(\sum_{i=1}^{n} a_i^p \right)^{1/p} \left(\sum_{i=1}^{n} a_i^q \right)^{1/q}$$

which holds for any non-negative real numbers a_i, b_i , $i = 1, 2, \ldots, n$. Setting $a_i = |\rho_i|^{2/3}$, $b_i = |\rho_i|^{4/3}$, $p = 3/2$, and $q = 3$, we obtain

$$\sum_{i=1}^{n} |\rho_i|^2 = \sum_{i=1}^{n} |\rho_i|^{2/3} \left(|\rho_i|^4 \right)^{1/3} \leq \left(\sum_{i=1}^{n} |\rho_i| \right)^{2/3} \left(\sum_{i=1}^{n} |\rho_i|^4 \right)^{1/3} . \tag{8}$$

If G has at least one edge, then not all ρ_i's are equal to zero. Then $\sum\limits_{i=1}^{n} |\rho_i|^4 \neq 0$ and (8) can be rewritten as

$$RE(G) = \sum_{i=1}^{n} |\rho_i| \geq \sqrt{\frac{\left(\sum\limits_{i=1}^{n} |\rho_i|^2 \right)^3}{\sum\limits_{i=1}^{n} |\rho_i|^4}} = \sqrt{\frac{\left(\sum\limits_{i=1}^{n} \rho_i^2 \right)^3}{\sum\limits_{i=1}^{n} \rho_i^4}}\ .$$

Theorem 5 is now obtained from Lemma 3. ■

Results analogous to Theorem 5 were earlier reported for the ordinary graph energy [38–41].

We conclude this section by a simple identity for the Randić energy of regular graphs.

Theorem 6. *If the graph G is regular of degree r , $r > 0$, then*

$$RE(G) = \frac{1}{r}\, E(G$$

If, in addition $r = 0$, then $RE = 0$.

Proof. If $r = 0$ then G is the graph without edges. Then directly from the definition (2) follows that $R_{ij} = 0$ for all $i, j = 1, 2, \ldots, n$, i. e., that $\mathbf{R}(G) = \mathbf{0}$. All eigenvalues of the zero matrix $\mathbf{0}$ are equal to zero. Therefore, $RE(G) = 0$.

Suppose now that G is regular of degree $r > 0$, i. e., that $d_1 = d_2 = \cdots = d_n = r$. Then all non-zero terms in $\mathbf{R}(G)$ are equal to $\frac{1}{r}$, implying that $\mathbf{R}(G) = \frac{1}{r}\,\mathbf{A}(G)$. Therefore, $\rho_i = \frac{1}{r}\,\lambda_i$ for $i = 1, 2, \ldots, n$. Theorem 6 follows from the definitions of E and RE , Eqs. (3) and (4). ∎

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