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Some Statistical Results on Randić Energy of Graphs

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Abstract

Let $\hat{G}_{n,m}$ be the set of all simple graphs with n vertices and m edges. In this paper, we establish the average value of the difference between Randić energy of two graphs selected randomly from the set $\hat{G}_{n,m}$. By means of this result, we get a criteria for deciding when two graphs are almost Randić equienergetic.

1 Introduction

The energy of a graph is defined as the sum of absolute values of its eigenvalues [13]. The motivation of the study of graph energy concept comes from chemistry, since there is a close relation between the graph energy and the total π-electron energy of a molecule represented by a (molecular) graph [11, 14].

Let G be a graph with n vertices, m edges and the vertex set $V(G) = \{1, 2, \ldots, n\}$. Use the notation $i \sim j$ if two vertices i and j of G are adjacent. Let d_i denotes the degree of the vertex i.

The adjacency matrix $A = A(G) = (a_{ij})$ of G is defined by $a_{ij} = 1$ if $i \sim j$ and 0 otherwise. Let $\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_n$ denote the eigenvalues of $A(G)$. These eigenvalues are said to be the eigenvalues of G and to form its spectrum [7]. Then the energy of G, denoted by E_G, is defined as [13]

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

For more information on the theory of $E(G)$, see the book [18] and the references cited therein.

Two non-isomorphic graphs are said to be cospectral if they have same eigenvalues [7]. Two graphs G_1 and G_2 are called equienergetic if their energies coincide, i.e., $E(G_1) = E(G_2)$ [2, 5, 12]. Obviously, cospectral graphs are equienergetic. Because of the existence of non-cospectral equienergetic graphs, equienergetic graphs recently have attracted great attention. The constructions of such graphs have been determined in [2, 5, 15, 17, 20, 24]. There also exists graphs whose energies are different, but remarkably close. These graphs are called almost equienergetic graphs [12, 20]. For more details on almost equienergetic graphs, see [12, 20, 22].

The Randić matrix $R = R(G) = (r_{ij})$ of G is defined as $r_{ij} = 1/\sqrt{d_i d_j}$ if $i \sim j$ and 0 otherwise [3]. Let $\rho_1 = 1 \geq \rho_2 \geq \cdots \geq \rho_n$ [19] be the eigenvalues of $R(G)$. These eigenvalues are called Randić eigenvalues of G. In full analogy with the ordinary graph energy (1), the Randić energy is defined as [3]

$$RE = RE(G) = \sum_{i=1}^{n} |\rho_i| . \tag{2}$$

Note that the Randić energy and the normalized Laplacian energy of graphs without isolated vertices coincide [3]. For the mathematical properties and the bounds on $RE(G)$, see [3, 4, 6, 8–10, 16].

Two non-isomorphic graphs are called Randić cospectral if they have same Randić eigenvalues [9]. Any two graphs G_1 and G_2 are said to be Randić equienergetic if $RE(G_1) = RE(G_2)$. These type of graphs are called in [1] Randić energy equivalent graphs. Throughout this paper, we prefer the notion Randić equienergetic. Randić cospectral graphs are clearly Randić equienergetic. Recently several Randić equienergetic graphs have been determined [21, 23]. In [21], a sequence of Randić equienergetic bipartite graphs was constructed. Tura [23] presented graphs both Randić non-cospectral and Randić equienergetic.

If the difference of the Randić energies of two graphs is very small, we call these graphs almost Randić equienergetic. In order to decide when the difference of Randić energies is very small, we need to know the average value of this difference. In this paper, we consider this problem. By means of the solution of the problem, we get a criteria for deciding when two graphs are almost Randić equienergetic.

2 Preliminaries and Results

In this section, we apply the same procedure as in [12] to Randić energy of graphs.

Let $\hat{G}_{n,m}$ be the set of all simple graphs with n vertices and m edges and let $G_1, G_2 \in \hat{G}_{n,m}$. The average value of the difference $|RE(G_1) - RE(G_2)|$, denoted by

$$\tilde{E}\left(|RE(G_1) - RE(G_2)|\right)$$

when the averaging is taken over all pairs of the elements of $\hat{G}_{n,m}$. Instead of it, we consider the closely similar quantity

$$\sqrt{\tilde{E}\left((RE(G_1) - RE(G_2))^2\right)} \tag{3}$$

whose statistical analysis is somewhat simpler. In fact, we have

$$\tilde{E}(RE(G_1)) = \tilde{E}(RE(G_2)) = \tilde{E}(RE)$$

and

$$\tilde{E}\left((RE(G_1))^2\right) = \tilde{E}\left((RE(G_2))^2\right) = \tilde{E}\left(RE^2\right).$$

We also have

$$\tilde{E}(RE(G_1) \cdot RE(G_2)) = \tilde{E}(RE(G_1)) \cdot \tilde{E}(RE(G_2)) = \left(\tilde{E}(RE)\right)^2$$

as $RE(G_1)$ and $RE(G_2)$ are considered as independent random variables. Then

$$\tilde{E}\left((RE(G_1) - RE(G_2))^2\right) = 2\left[\tilde{E}\left(RE^2\right) - \left(\tilde{E}(RE)\right)^2\right] \tag{4}$$

where $\tilde{E}(RE)$ and $\tilde{E}(RE^2)$ denote the average value of Randić energy and its square, respectively, averaged over all elements in $\hat{G}_{n,m}$

We first give an approximate relation between $\tilde{E}(RE)$ and $\tilde{E}(RE^2)$. For this, we suppose that in our statistical considerations, the Randić eigenvalues $\rho_1, \rho_2, \ldots, \rho_n$ are replaced by the random variables $x_1, x_2, \ldots, x_n$ with an arbitrary probability distribution which is the same for each x_i.

Theorem 1. *Let $\tilde{E}(RE)$ and $\tilde{E}(RE^2)$ be the average value of Randić energy and its square, respectively. Then $\tilde{E}(RE)$ and $\tilde{E}(RE^2)$ are approximately related as:*

$$\tilde{E}\left(RE^2\right) \approx 2R_{-1} + \frac{n-1}{n}\left(\tilde{E}(RE)\right)^2 \tag{5}$$

where

$$R_{-1} = \sum_{i \sim j} \frac{1}{d_i d_j}.$$

Proof. By taking the average value of the square of Randić energy,

$$\begin{aligned}\tilde{E}\left(RE^2\right) &= \tilde{E}\left(\left(\sum_{i=1}^{n}|\rho_i|\right)^2\right) = \tilde{E}\left(\sum_{i=1}^{n}\rho_i^2 + 2\sum_{i<j}|\rho_i|\,|\rho_j|\right)\\ &= 2R_{-1} + 2\left(\sum_{i<j}\tilde{E}\left(|\rho_i|\right)\tilde{E}\left(|\rho_j|\right)\right),\end{aligned}$$

since for all graphs in $\hat{G}_{n,m}$ [3]

$$\sum_{i=1}^{n}\rho_i^2 = 2\sum_{i\sim j}\frac{1}{d_i\,d_j}. \tag{6}$$

Replacing ρ_i and ρ_j by x_i and x_j and taking into account that these two variables are statistically independent such that $\tilde{E}\left(|x_i|\right) = \tilde{E}\left(|x_j|\right) = \tilde{E}\left(|x|\right)$, we arrive at

$$\begin{aligned}\tilde{E}\left(RE^2\right) &\approx 2R_{-1} + 2\left(\sum_{i<j}\tilde{E}\left(|x_i|\right)\tilde{E}\left(|x_j|\right)\right)\\ &= 2R_{-1} + 2\left(\sum_{i<j}\tilde{E}\left(|x|\right)^2\right)\\ &= 2R_{-1} + \frac{n-1}{n}\left(n\tilde{E}\left(|x|\right)\right)^2. \end{aligned}\tag{7}$$

Note that

$$\tilde{E}\left(RE\right) = \tilde{E}\left(\sum_{i=1}^{n}|\rho_i|\right) = \sum_{i=1}^{n}\tilde{E}\left(|\rho_i|\right) \approx \sum_{i=1}^{n}\tilde{E}\left(|x_i|\right) = n\tilde{E}\left(|x|\right). \tag{8}$$

Thus by (7) and (8),

$$\tilde{E}\left(RE^2\right) \approx 2R_{-1} + \frac{n-1}{n}\left(\tilde{E}\left(RE\right)\right)^2$$

which is the required result. ■

Note that, in relation (5), R_{-1} denotes the well known graph quantity which is called general Randić index [6].

Relation (5) has been obtained without specifying the actual distribution of the random variables $x_1, x_2, \ldots, x_n$. If we want to obtain the average difference (3) from (4) and (5), then we must know this distribution, at least approximately. In order to do this, we use the probability function of the random variables $x_1, x_2, \ldots, x_n$. Let $\Gamma\left(x\right)$ denote such a function. Using this function, we give a statistical model for the actual distribution of the Randić eigenvalues of the graphs in $\hat{G}_{n,m}$. Note that the function $\Gamma\left(x\right)$ has the following conditions [12]:

$$\Gamma\left(x\right) \geq 0, \text{ for all } x \in (-\infty, +\infty) \tag{9}$$

and

$$\int_{-\infty}^{+\infty} \Gamma(x)\, dx = 1. \tag{10}$$

We require that

$$\int_{-\infty}^{+\infty} x\, \Gamma(x)\, dx = 0. \tag{11}$$

as $\sum_{i=1}^{n} \rho_i = 0$ [3]. Then, from (2) and (8)

$$\tilde{E}(RE) = n \int_{-\infty}^{+\infty} |x|\ \Gamma(x)\, dx. \tag{12}$$

Graovac et al. [12] considered two models for $\Gamma(x)$ and determined the average value of the difference between the energy of the graphs G_1 and G_2, denoted by $\tilde{E}(|E(G_1) - E(G_2)|)$, randomly chosen from the set $\hat{G}_{n,m}$. The first model for $\Gamma(x)$ was given by the following uniform–distribution [12]

$$\Gamma(x_i) = \Gamma(x) = \begin{cases} 1/(2\alpha) & \text{if } |x| \leq \alpha \\ 0 & \text{if } |x| > \alpha \end{cases} \tag{13}$$

The second model for $\Gamma(x)$ was given as [12]

$$\Gamma(x_i) = \Gamma(x) = \begin{cases} h_\beta & \text{if } -\beta \leq x \leq 0 \\ h_\alpha & \text{if } 0 < x \leq \alpha \\ 0 & \text{otherwise} \end{cases} \tag{14}$$

For $\alpha = \beta$ the model (14) is reduced to the model (13) [12].

Remark 1. *By means of the model (13), Graovac et al. [12] gave the following estimation of the average difference of graph energies:*

$$\tilde{E}(|E(G_1) - E(G_2)|) \approx \sqrt{m}. \tag{15}$$

From the model in (14), they obtained that [12]

$$\tilde{E}(|E(G_1) - E(G_2)|) \approx \sqrt{m - \frac{10mnt^2}{3m^3 + 2nt^2}} \tag{16}$$

where t is the average number of triangles of the graphs in the set $\hat{G}_{n,m}$. From the above results, they concluded that because of the existence of triangles in (some) graphs, the average difference of graph energies (16) is somewhat smaller than (15). They also

pointed out that (16) is reduced to (15) when $t = 0$. Unfortunately, there is a small mistake in the calculation of (16). Taking into account the procedure in [12], we have

$$\tilde{E}\left(\left|E\left(G_1\right) - E\left(G_2\right)\right|\right) \approx \sqrt{m + \frac{6mnt^2}{3m^3 + 2nt^2}}$$

This states that because of the existence of triangles in (some) graphs, the average difference of graph energies (16) gives somewhat greater estimation than (15).

Theorem 2. *Let G_1 and G_2 be two graphs randomly chosen from the set $\hat{G}_{n,m}$. Then*

$$\tilde{E}\left(\left|RE\left(G_1\right) - RE\left(G_2\right)\right|\right) \approx \sqrt{R_{-1}} \tag{17}$$

where

$$R_{-1} = \sum_{i \sim j} \frac{1}{d_i\, d_j}.$$

Proof. In the proof, we use the model (13) for $\Gamma(x)$ which satisfies the conditions (9)–(11) [12]. Note that the parameter α in (13) is determined with the condition

$$\int_{-\infty}^{+\infty} x^2\, \Gamma(x)\, dx = \frac{2R_{-1}}{n}. \tag{18}$$

which gives just a reformulation of (6). In (18), R_{-1} must be considered as the average general Randić index of the graphs in the set $\hat{G}_{n,m}$. By (12),(13), and (18), we directly get that $\alpha = \sqrt{\frac{6R_{-1}}{n}}$ and

$$\tilde{E}\left(RE\right) = \frac{\sqrt{3}}{2}\sqrt{2nR_{-1}}. \tag{19}$$

Then by (4), (5) and (19),

$$\begin{aligned}
\tilde{E}\left(\left(RE\left(G_1\right) - RE\left(G_2\right)\right)^2\right) &= 2\left(\tilde{E}\left(RE^2\right) - \left(\tilde{E}\left(RE\right)\right)^2\right) \\
&\approx 2\left(2R_{-1} + \frac{n-1}{n}\left(\tilde{E}\left(RE\right)\right)^2 - \left(\tilde{E}\left(RE\right)\right)^2\right) \\
&= 4R_{-1} - \frac{2}{n}\left(\tilde{E}\left(RE\right)\right)^2 = R_{-1}.
\end{aligned}$$

Thus

$$\tilde{E}\left(\left|RE\left(G_1\right) - RE\left(G_2\right)\right|\right) \approx \sqrt{R_{-1}}$$

which is the required result. ■

Theorem 3. *Let G_1 and G_2 be two graphs randomly chosen from the set $\hat{G}_{n,m}$. Then*

$$\tilde{E}\left(\left|RE\left(G_1\right)-RE\left(G_2\right)\right|\right)\approx\sqrt{R_{-1}+\frac{3nR_{-1}T^2}{nT^2+54\left(R_{-1}\right)^3}}. \tag{20}$$

where

$$R_{-1}=\sum_{i\sim j}\frac{1}{d_i\,d_j}\qquad\text{and}\qquad T=2\sum_{i\sim j}\frac{1}{d_i\,d_j}\left(\sum_{k\sim i,k\sim j}\frac{1}{d_k}\right).$$

Proof. In this proof, we use the model (14) for $\Gamma(x)$. Note that the parameters α,β,h_α and h_β in (14) are determined by the conditions (10), (11), (18), and (21)

$$\int_{-\infty}^{+\infty}x^3\,\Gamma(x)\,dx=\frac{T}{n}. \tag{21}$$

Note that (21) is a reformulation of the following identity obtained in [3]

$$\sum_{i=1}^{n}\rho_i^3=2\sum_{i\sim j}\frac{1}{d_i\,d_j}\left(\sum_{k\sim i,k\sim j}\frac{1}{d_k}\right). \tag{22}$$

In (21) the parameter T must be considered as the average T value of the graphs in $\hat{G}_{n,m}$. From (10) and (11), it was obtained that [12]

$$h_\alpha=\frac{\beta}{\alpha\left(\alpha+\beta\right)}\quad;\quad h_\beta=\frac{\alpha}{\beta\left(\alpha+\beta\right)}.$$

Considering (18) and (21), we get

$$\alpha\beta=\frac{6R_{-1}}{n}\quad;\quad\alpha-\beta=\frac{2T}{3R_{-1}} \tag{23}$$

from which we have

$$\alpha=\frac{T}{3R_{-1}}+\sqrt{\frac{T^2}{9\left(R_{-1}\right)^2}+\frac{6R_{-1}}{n}}\quad;\quad\beta=-\frac{T}{3R_{-1}}+\sqrt{\frac{T^2}{9\left(R_{-1}\right)^2}+\frac{6R_{-1}}{n}}. \tag{24}$$

By (12), (23), and (24), we obtain

$$\tilde{E}\left(RE\right)=3R_{-1}\left(\frac{T^2}{9\left(R_{-1}\right)^2}+\frac{6R_{-1}}{n}\right)^{-1/2}.$$

Combining this result with (4) and (5), we arrive at

$$\tilde{E}\left(\left(RE\left(G_1\right)-RE\left(G_2\right)\right)^2\right)\approx R_{-1}+\frac{3nR_{-1}T^2}{nT^2+54\left(R_{-1}\right)^3}.$$

Thus

$$\tilde{E}\left(\left|RE\left(G_1\right)-RE\left(G_2\right)\right|\right)\approx\sqrt{R_{-1}+\frac{3nR_{-1}T^2}{nT^2+54\left(R_{-1}\right)^3}}.$$

This completes the proof. ■

Remark 2. *Note that for bipartite graphs of order n, $\rho_i = -\rho_{n-i+1}$ for $i = 1, 2, \ldots \left\lceil \frac{n}{2} \right\rceil$ [10]. Then we conclude that for bipartite graphs in $\hat{G}_{n,m}$ (20) is reduced to (17) as $T = 0$. Further note that for non-bipartite graphs $T \neq 0$ in which case (17) gives better estimation than (20) for the average value of the difference between Randić energy of two graphs.*

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