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New Bounds on the Normalized Laplacian (Randić) Energy

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Abstract

In this paper, we consider the energy of a simple graph with respect to its normalized Laplacian eigenvalues (Randić eigenvalues), which we call the normalized Laplacian energy (also Randić energy). We provide improved upper and lower bounds on these energies for connected (bipartite) graphs.

1 Introduction and preliminaries

Let G be a finite, simple and undirected graph with n vertices. Let $V(G) = \{v_1, v_2, ..., v_n\}$ be the vertex set of G. If any vertices v_i and v_j are adjacent, then we use the notation $v_i \sim v_j$. For $v_i \in V(G)$, the degree of the vertex v_i, denoted by d_i, is the number of the vertices adjacent to v_i.

The matrix $L(G) = D(G) - A(G)$ is called the Laplacian matrix [27, 28] of G, where $A(G)$ is the adjacency matrix and $D(G)$ is the diagonal matrix of the vertex degrees. Since $A(G)$ and $L(G)$ are all real symmetric matrices, their eigenvalues are real numbers. So, we can assume that $\lambda_1(G) \geq \lambda_2(G) \geq ... \geq \lambda_n(G)$ ($\mu_1(G) \geq \mu_2(G) \geq ... \geq \mu_n(G) = 0$) are the adjacency (Laplacian) eigenvalues of G. It follows from the Geršgorin disc theorem that $L(G)$ is semidefinite. Therefore, all Laplacian eigenvalues of

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G are nonnegative. If the graph G is a connected non-bipartite graph, then $\mu_i(G) > 0$ for $i = 1, 2, ..., n$ [10]. Because the graph G is assumed to be connected, it has no isolated vertices (i.e., $d_i > 0$ for all $1 \le i \le n$) and therefore the matrix $D^{-1/2}(G)$ is well-defined. Then $L^* = L^*(G) = D^{-1/2}(G)\, L(G)\, D^{-1/2}(G)$ is called the normalized Laplacian matrix of the graph G. Its eigenvalues are $\rho_1(G) \ge \rho_2(G) \ge ... \ge \rho_n(G) = 0$. For details of the spectral theory of the normalized Laplacian matrix, see [7].

It is convenient to write the normalized Laplacian matrix as $I_n - R$, where $R = R(G)$ is the so-called Randić matrix whose (i,j)-entry is

$$\mathbf{r}_{ij} = \begin{cases} \frac{1}{\sqrt{d_i d_j}}, & \text{if } v_i \sim v_j \\ 0, & \text{otherwise} . \end{cases}$$

The Randić eigenvalues $q_1, q_2, ..., q_n$ of the graph G are the eigenvalues of its Randić matrix. Since $R(G)$ is a real symmetric matrix, its eigenvalues are real numbers. So we can order them so that $q_1 \ge q_2 \ge ... \ge q_n$.

One of the most remarkeble chemical applications of graph theory is based on the close-correspondence between the graph eigenvalues and the molecular orbital energy levels of $\pi-$electrons in conjugated hydrocarbons. For the Hüchkel molecular orbital approximation, the total $\pi-$electron energy in conjugated hydrocarbons is given by the sum of absolute values of the eigenvalues corresponding to the molecular graph G in which the maximum degree is not more than four in general.

The singular values of a real matrix (not necessarily square) M are the square roots of the eigenvalues of the matrix MM^T, where M^T denotes the transpose of M.

For convenience, if M is a real symmetric matrix of order n, we order and denote the eigenvalues by $\lambda_1(M) \ge \lambda_2(M) \ge ... \ge \lambda_n(M)$ and the singular values by $\sigma_1(M) \ge \sigma_2(M) \ge ... \ge \sigma_n(M)$. Nikiforov [29] extended the concept of graph energy to any matrix M, *i.e.*, if G is a graph and M is a real symmetric matrix associated with G, then the $M-$energy of G is

$$E_M(G) = \sum_{i=1}^{n} \left| \lambda_i(M) - \frac{tr(M)}{n} \right|, \tag{1}$$

where $tr(M)$ is the trace of M.

The energy of G was defined by Gutman in [13, 14] as

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

Research on graph energy is nowadays very active, as seen from the recent papers [21]-[23], [25], [29]-[32], [15, 17] monograph [23], the references quoted therein. Recently, the Laplacian energy [16, 33], Randić energy [2]-[4],[8, 18, 12], [24], [26] and the normalized Laplacian energy [6, 19, 20] of a graph has received much interest. Along the same lines, the energy of more general matrices and sequences has been studied.

Using (1) with M taken to be L^*, the normalized Laplacian energy and Randić energy of a graph G is

$$E_{L^*}(G) = \sum_{i=1}^{n} |\rho_i - 1| = \sum_{i=1}^{n} |\lambda_i (I_n - L^*)| \quad \text{and} \quad E_R(G) = \sum_{i=1}^{n} |q_i| . \tag{2}$$

Since $L^* = I_n - R$, it is easy to see that this equivalent to

$$E_{L^*}(G) = \sum_{i=1}^{n} |q_i| = \sum_{i=1}^{n} \sigma_i (R) = E_R(G) .$$

Some basic properties of $E_{L^*}(G)$ may be found in [6].

From (1), one can immediately get the normalized Laplacian energy of a graph by computing the normalized Laplacian eigenvalues of the graph. However, even for special graphs, it is still complicated to find the normalized Laplacian eigenvalues of them. Hence, it makes sense to establish lower and upper bounds to estimate the invariant for some classes of graphs.

Recall that the general Randić index of a graph G is defined in [1] as

$$R_\alpha = R_\alpha(G) = \sum_{v_i \sim v_j} (d_i d_j)^\alpha ,$$

where $\alpha \neq 0$ is a fixed real number.

The general Randić index when $\alpha = -1$ is

$$R_{-1} = R_{-1}(G) = \sum_{v_i \sim v_j} \frac{1}{d_i d_j} .$$

Some properties on R_{-1} can be founded in [6].

The complete product $G_1 \vee G_2$ of graphs G_1 and G_2 is the graph obtained from $G_1 \cup G_2$ by joining every vertex of G_1 with every vertex of G_2. Generally, we denote by K_n and $K_{p,q}$ $(p + q = n)$ the complete graph and complete bipartite graph.

Gutman et al. [19] gave lower bound for normalized Laplacian energy using the Randic index. In [6], Cavers et al. obtained lower and upper bounds for $E_{L^*}(G)$. In addition, some bounds were obtained for $E_{L^*}(G)$ by Hakimi-Neshaad in [20].

We purpose to obtain some better bounds using the following inequality (in Lemma 1.1) technique on our main results.

Lemma 1.1 *[33] Let $a_1, a_2, ..., a_n$ be nonnegative numbers. Then*

$$\begin{aligned} n\left[\frac{1}{n}\sum_{i=1}^{n} a_i - \left(\prod_{i=1}^{n} a_i\right)^{1/n}\right] &\leq n\sum_{i=1}^{n} a_i - \left(\sum_{i=1}^{n}\sqrt{a_i}\right)^2 \\ &\leq n(n-1)\left[\frac{1}{n}\sum_{i=1}^{n} a_i - \left(\prod_{i=1}^{n} a_i\right)^{1/n}\right]. \end{aligned}$$

In this paper, we obtain some new bounds on $E_{L^*}(G) (= E_R(G))$ of graphs and improve some results which were obtained on this energies. In the following we recall some results from spectral graph theory, and state a few analytical inequalities for our work.

Lemma 1.2 *[7] Let the normalized Laplacian eigenvalues of G be given as $\rho_1 \geq \rho_2 \geq .... \geq \rho_n = 0$. Then*

$$0 \leq \rho_i \leq 2.$$

Morever $\rho_1 = 2$ if and only if G has a connected bipartite and nontrivial component.

Lemma 1.3 *[34] Let G be an undirected, simple and connected graph with n, $n \geq 2$, vertices and m edges. Then*

$$\sum_{i=1}^{n-1} \rho_i = n \quad \textit{and} \quad \sum_{i=1}^{n} \rho_i^2 = n + 2R_{-1}$$

where $R_{-1} = \sum_{v_i \sim v_j} \frac{1}{d_i d_j}$.

Lemma 1.4 *[31] Let G be a graph of order n with no isolated vertices. Suppose G has minimum vertex degree equal to $d_{\min}$ and maximum vertex degree equal to $d_{\max}$. Then*

$$\frac{n}{2d_{\max}} \leq R_{-1} \leq \frac{n}{2d_{\min}}.$$

Equality occurs in both bounds if and only if G is a regular graph.

Theorem 1.5 *[9] Let G be a connected graph of order n and Δ be the absolute value of the determinant of the Randic matrix $R(G)$. Then*

$$E_R(G) = \begin{cases} \geq 1 + \sqrt{2R_{-1} - 1 + (n-1)(n-2)\Delta^{2/(n-1)}} \\ \leq 1 + \sqrt{(n-1)(2R_{-1} - 1)}. \end{cases}$$

If the maximum degree $d_{\max}$ is equal to $n-1$, then both the equalities hold if and only if $G \cong K_n$ or $G \cong K_1 \vee rK_2$ with $n = 2r + 1$ $(r \geq 2)$.

2 Main Results

After all above materials, we are ready to present our main results.

Theorem 2.1 *Let G be an undirected, simple and connected graph with $n, n \geq 3$ vertices. Then*

$$E_{L^*}(G) = E_R(G) = \begin{cases} \geq 1 + \sqrt{2R_{-1} - 1 + (n-1)(n-2)\Delta^{2/(n-1)}} \\ \leq 1 + \sqrt{(n-2)(2R_{-1} - 1) + (n-1)\Delta^{2/(n-1)}} \end{cases} \tag{3}$$

where $\Delta = \det(I_n - L^*)$. If the maximum degree $d_{\max}$ is equal to $n-1$, then both the equalities hold if and only if $G \cong K_n$ or $G \cong K_1 \vee rK_2$ with $n = 2r+1$ $(r \geq 2)$.

Proof. Setting $a_i = (\rho_i - 1)^2$ and replacing n by $n-1$ in Lemma 1.1, we obtain that

$$\mathbf{N} \leq (n-1)\sum_{i=1}^{n-1}(\rho_i - 1)^2 - \left(\sum_{i=1}^{n-1}|\rho_i - 1|\right)^2 \leq (n-2)\,\mathbf{N},$$

where $\mathbf{N} = (n-1)\left[\frac{1}{n-1}\sum_{i=1}^{n-1}(\rho_i - 1)^2 - \left(\prod_{i=1}^{n-1}(\rho_i - 1)^2\right)^{1/(n-1)}\right]$.

Therefore, considering Lemma 1.3 we have

$$\mathbf{N} \leq (n-1)(2R_{-1} - 1) - (E_{L^*}(G) - 1)^2 \leq (n-2)\,\mathbf{N}.$$

Observe that

$$\begin{aligned} \mathbf{N} &= (n-1)\left[\frac{1}{n-1}\sum_{i=1}^{n-1}(\rho_i - 1)^2 - \left(\prod_{i=1}^{n-1}(\rho_i - 1)^2\right)^{1/(n-1)}\right] \\ &= (n-1)\left[\frac{1}{n-1}(2R_{-1} - 1) - \left(\prod_{i=1}^{n-1}(\rho_i - 1)\right)^{2/(n-1)}\right] \\ &= 2R_{-1} - 1 - (n-1)\Delta^{2/(n-1)}. \end{aligned}$$

Hence we get result. For equality conditions, it can be seen in Theorem 1.5. ■

Remark 2.2 *In [20], Hakiminezhaad and Ashrafi obtained the following lower bound for the normalized Laplacian energy :*

$$E_{L^*}(G) \geq 1 + \sqrt{\frac{n}{d_{\max}} - 1 + 2\binom{n-1}{2}\Delta^{2/(n-1)}}. \tag{4}$$

From Lemma 1.4, the lower bound (3) is better than the lower bound (4).

A strongly regular graph with parameters (n,r,λ,μ), denoted by $SRG(n,r,\lambda,\mu)$, is an $r-$regular graph on n vertices such that for every pair of adjacent vertices there are λ vertices adjacent to both, and for every pair of non-adjacent vertices there are μ vertices adjacent to both.

Considering Lemma 1.4 and the inequality (3), we arrive at the following result.

Corollary 2.3 *Let G be a graph of order n with no isolated vertices. Suppose G has minimum vertex degree equal to $d_{\min}$ and maximum vertex degree equal to $d_{\max}$. Then*

$$E_{L^*}(G) = E_R(G) = \begin{cases} \geq 1 + \sqrt{\frac{n}{d_{\max}} - 1 + (n-1)(n-2)\Delta^{2/(n-1)}} \\ \leq 1 + \sqrt{(n-2)\left(\frac{n}{d_{\min}} - 1\right) + (n-1)\Delta^{2/(n-1)}} \end{cases} \tag{5}$$

where $\Delta = \det(I_n - L^*)$. Equality holding in both of these inequalities if and only if $G \cong SRG\left(n, \delta, \frac{\delta^2-\delta}{n-1}, \frac{\delta^2-\delta}{n-1}\right)$ or $G \cong K_n$.

In (5), in the upside, one of the present authors [8] gave the proof the equality holding if and only if $G \cong SRG\left(n, \delta, \frac{\delta^2-\delta}{n-1}, \frac{\delta^2-\delta}{n-1}\right)$ or $G \cong K_n$. Morever, these characterizations of extremal graphs are also satisfying for the underside equality.

Remark 2.4 *It can be easy to see that the bound (3) is better than all results which were obtained for $E_{L^*}(G)$ in [19] and [6] on many examples. We consider the graph $G = (V,E)$ with vertex set $V = \{v_1, v_2, v_3, v_4\}$ and the edge set $E = \{v_1v_2, v_2v_3, v_1v_3, v_3v_4\}$. For this graph, $E_{L^*}(G) = 2.4574$. While the lower bound in (3) gives $E_{L^*}(G) \geq 2.406$, the lower bounds in Theorem 16 [6] and (3.8) [19], give $E_{L^*}(G) \geq 2.3016$ and $E_{L^*}(G) \geq 1$, respectively.*

Similarly, while the upper bound in (3) gives $E_{L^*}(G) \leq 2.49$, the upper bound in Lemma1 [6] gives $E_{L^*}(G) \leq 2.708$.

If G has k connected components, in particular, $G_1, G_2, ..., G_k$, then

$$E_{L^*}(G) = \sum_{i=1}^{k} E_{L^*}(G_i) \ .$$

We first provide a bound on the normalized Laplacian energy of a graph with k components.

Theorem 2.5 *Let G be a graph of order n with k connected components and with no isolated vertices. Then*

$$E_{L^*}(G) = E_R(G) = \begin{cases} \geq k + \sqrt{2R_{-1} - k + (n-k-1)(n-k)\Delta^{2/(n-k)}} \\ \leq k + \sqrt{(n-k-1)(2R_{-1} - k) + (n-k)\Delta^{2/(n-k)}} \end{cases} \tag{6}$$

where $\Delta = \det(I_n - L^*)$.

Proof. Note that 0 is an eigenvalue of L^* with multiplicity k. The rest of the proof is similar to the proof of Theorem 2.1, replacing n by $n-k$. ∎

Using the bounds of R_{-1} in the above Lemma 1.4, we give the following corollary.

Corollary 2.6 *Let G be a graph of order n with k connected components and with no isolated vertices. Then*

$$E_{L^*}(G) = E_R(G) = \begin{cases} \geq k + \sqrt{\frac{n}{d_{\max}} - k + (n-k-1)(n-k)\Delta^{2/(n-k)}} \\ \leq k + \sqrt{(n-k-1)\left(\frac{n}{d_{\min}} - k\right) + (n-k)\Delta^{2/(n-k)}} \end{cases}.$$

Taking $k=2$ in (6),we obtain the following result for the normalized Laplacian energy (Randić energy) of connected bipartite graphs.

Corollary 2.7 *Let G be a connected bipartite graph with $n \geq 3$ vertices. Then*

$$E_{L^*}(G) = E_R(G) = \begin{cases} \geq 2 + \sqrt{2R_{-1} - 2 + (n-2)(n-3)\Delta^{2/(n-2)}} \\ \leq 2 + \sqrt{(n-3)(2R_{-1} - 2) + (n-2)\Delta^{2/(n-2)}} \end{cases} \tag{7}$$

with equality holding for odd n in both of these inequalities if and only if $G \cong K_{p,q}$ with $n = p+q$.

Proof. Since G is bipartite, we have $\rho_1 = 2$ [7]. Then, if we combine this fact with the proof of Theorem 2.5 , we arrive at the result. One can easily check that both equalities hold if and only if G is bipartite graph with

$$|\rho_2 - 1| = |\rho_3 - 1| = ... = |\rho_{n-1} - 1| = \sqrt{\frac{2R_{-1} - 2}{n-2}}.$$

If $\rho_2 = 1$, then $G \cong K_{p,q}$ with $n = p+q$. Otherwise $\rho_2 > 1$. Since G is bipartite graph, one can easily see that G is a bipartite graph with normalized Laplacian spectrum

$$\left\{ 2, \underbrace{1 \pm \sqrt{\frac{2R_{-1} - 2}{n-2}}, ..., 1 \pm \sqrt{\frac{2R_{-1} - 2}{n-2}}}_{\frac{n-2}{2}}, 0 \right\}.$$

∎

Using the bounds of R_{-1} in the Corollary 2.7, we give the following result. For equality conditions, it can be seen in [8].

Corollary 2.8 *Let G be a connected bipartite graph with $n \geq 3$ vertices. Then*

$$E_{L^*}(G) = E_R(G) = \begin{cases} \geq 2 + \sqrt{\frac{n}{d_{\max}} - 2 + (n-2)(n-3)\Delta^{2/(n-2)}} \\ \leq 2 + \sqrt{(n-3)\left(\frac{n}{d_{\min}} - 2\right) + (n-2)\Delta^{2/(n-2)}} \end{cases} \tag{8}$$

with equality holding in both of these inequalities if and only if $G \cong K_{\nu,\nu}$ or G is the incidence graph of a symmetric $2-\left(\nu, d_{\min}, \frac{2d_{\min}^2 - 2d_{\min}}{n-2}\right)-$design [11] (see, p.166) where $n = 2\nu$ and $\nu > d_{\min}$.

Remark 2.9 *Recently, the concept of Randić energy was studied intensively in the literature. One can easily see that the bound (3) is better than the some previous results.*

For example, the lower bound which was obtained for Randić energy in [8] is the same with the bound (5). But we know that (3) is better than (5). In addition, the lower bound in [26] is also same with the bound (3). Again, in [5], [24], [26] it was presented the following upper bound for Randić energy

$$E_R(G) \leq 1 + \sqrt{(n-1)(2R_{-1} - 1)}. \tag{9}$$

Using the arithmetic-geometric mean inequality, it follows that the upper bound in (3) is better than the upper bound (9). Similarly, the upper bounds (7) and (8) over Randić energy of connected bipartite graphs are better than the results which were obtained in [9].

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