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RANDIĆ INDEX AND EIGENVALUES OF GRAPHS

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ABSTRACT. Let G be a simple connected graph. The general Randić index $R_\alpha(G)$ of G is defined as $R_\alpha(G) = \Sigma_{uv \in E(G)}(d(u)\,d(v))^\alpha$. In this paper, we present upper and lower bounds for $R_{-1}(G)$ in terms of the normalized Laplacian eigenvalues of a graph.

1. Introduction. In this paper, we use the standard notation in graph theory in [**4**]. Let $G = (V(G), E(G))$ be a simple connected graph with vertex set $V(G)$ and edge set $E(G)$, $|V(G)| = n$ and $|E(G)| = m$. The general Randić index $R_\alpha(G)$ of G is defined as the sum of $(d_u d_v)^\alpha$ over all edges uv of G, where d_u denotes the degree of $u \in V(G)$, i.e.,

$$R_\alpha(G) = \Sigma_{uv \in E(G)}(d_u d_v)^\alpha,$$

where α is an arbitrary real number.

It is well known that $R_{-1/2}$ was introduced by Randić in 1975 as one of the many graph theoretical parameters derived from the graph underlying some molecule [**13**]. Like other successful chemical indices, this has been closely correlated with many chemical properties. The general Randić index was proposed by Bollobás and Erdös [**3**], and Amic et al. [**1**], independently, in 1998. It has been extensively studied by both mathematicians and theoretical chemists. Many important mathematical properties have been established. Li and Yang [**11**] studied the general Randić index for general graphs and obtained lower and upper bounds for the general Randić index among graphs of order n. Araujo et al. [**2**], Lu et al. [**12**], Gutman et al. [**6, 7**] and Xiao et al. [**14**] studied the general Randić index in terms of eigenvalues of the Laplacian matrix and the adjacent matrix of a graph. Later Hu

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et al. [**8, 9**] studied the trees with extremal general Randić index. Zhang et al. [**15**] studied the maximum Randić index for trees with k pendent vertices. For a survey of related results, we refer to the new book written by Li and Gutman [**10**].

In [**5**], Fan Chung defined the *normalized Laplacian* matrix $L(G) = (L_{uv})_{n\times n}$ of a graph G as follows:

$$L_{uv} = \begin{cases} 1 & \text{if } u = v \text{ and } d_u \neq 0; \\ -1/\sqrt{d_u d_v} & \text{if } u \sim v; \\ 0 & \text{otherwise,} \end{cases}$$

where d_u is the degree of vertex u.

It is well known that $L(G)$ is real and positive semi-definite and that its eigenvalues are all real and nonnegative. We call eigenvalues of $L(G)$ the *normalized Laplacian eigenvalues* of G, and the eigenvalues of $L(G)$ are ordered by $\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_{n-1} \geq \lambda_n = 0$. The matrix $A(G)$ is the adjacency matrix of graph G; we use $\rho(G)$ to denote the spectral radius of $A(G)$.

The focus of this paper is on the bounds for $R_{-1}(G)$ of graphs by means of normalized Laplacian eigenvalues. In fact, we get the following results.

Theorem 1.1. *Let G be a simple connected graph on n vertices. Then*

$$(1) \qquad R_{-1}(G) \leq \frac{1}{2}(n-1)(n-2)\left(\lambda_1 - \frac{n}{n-1}\right)^2 + \frac{n}{2(n-1)},$$

$$(2) \qquad R_{-1}(G) \leq \frac{1}{2}(n-1)(n-2)\left(\lambda_{n-1} - \frac{n}{n-1}\right)^2 + \frac{n}{2(n-1)},$$

with equalities holding if and only if $G \cong K_n$.

Theorem 1.2. *Let G be a simple connected graph on n vertices. If $\rho(G) \leq 2/(\sum_{u\in V(G)} d_u^{-2})$, then*

$$(3) \qquad R_{-1}(G) > \frac{n-1}{2(n-2)}\left(\lambda_1 - \frac{n}{n-1}\right) + \frac{n}{2(n-1)}.$$

2. Lemmas and results. In order to prove Theorems 1.1 and 1.2, we need some technical lemmas.

Lemma 2.1 [**5**]. *Let G be a graph on n vertices. Then, for $n \geq 2$,*

$$\lambda_{n-1} \leq \frac{n}{n-1}, \tag{4}$$

$$\lambda_1 \geq \frac{n}{n-1}. \tag{5}$$

The equalities in (4) *and* (5) *hold if and only if $G \cong K_n$.*

Lemma 2.2. *Let $G = G(n,m)$ be a simple connected graph on n vertices. Then*

$$\lambda_1 \geq \frac{n}{n-1} + \sqrt{\frac{1}{(n-1)(n-2)}\left(2\sum_{u\sim v}\frac{1}{d_u d_v} - \frac{n}{n-1}\right)}, \tag{6}$$

$$\lambda_{n-1} \leq \frac{n}{n-1} - \sqrt{\frac{1}{(n-1)(n-2)}\left(2\sum_{u\sim v}\frac{1}{d_u d_v} - \frac{n}{n-1}\right)}, \tag{7}$$

with equalities in (6) *and* (7) *holding if and only if G is a complete graph.*

Proof. It is obvious that, for a fixed k,

$$\begin{aligned}\left[\sum_{i=1}^{n-1}(\lambda_i) - (n-1)\lambda_k\right]^2 \\ &= \left[\sum_{i=1}^{n-1}(\lambda_i - \lambda_k)\right]^2 \\ &= \sum_{i=1}^{n-1}(\lambda_i - \lambda_k)^2 + 2\sum_{1\leq i<j\leq n-1}(\lambda_i - \lambda_k)(\lambda_j - \lambda_k).\end{aligned}$$

Particularly, when $k = 1$, or $n-1$,

$$\sum_{1\leq i<j\leq n-1}(\lambda_i - \lambda_k)(\lambda_j - \lambda_k) \geq 0. \tag{8}$$

So we have

$$\left[\sum_{i=1}^{n-1}(\lambda_i)-(n-1)\lambda_k\right]^2 \geq \sum_{i=1}^{n-1}(\lambda_i-\lambda_k)^2.$$

Thus,

$$\left(\sum_{i=1}^{n-1}\lambda_i\right)^2-2(n-1)\lambda_k\sum_{i=1}^{n-1}\lambda_i+(n-1)^2\lambda_k^2 \\ \geq \sum_{i=1}^{n-1}\lambda_i^2-2\lambda_k\sum_{i=1}^{n-1}\lambda_i+(n-1)\lambda_k^2.$$

This is equivalent to

$$\lambda_k^2-2\frac{1}{n-1}\lambda_k\sum_{i=1}^{n-1}\lambda_i+\frac{1}{(n-1)^2-(n-1)}\left(\sum_{i=1}^{n-1}\lambda_i\right)^2 \\ \geq \frac{1}{(n-1)^2-(n-1)}\sum_{i=1}^{n-1}\lambda_i^2,$$

or

$$\left(\lambda_k-\frac{1}{n-1}\sum_{i=1}^{n-1}\lambda_i\right)^2-\frac{1}{(n-1)^2}\left(\sum_{i=1}^{n-1}\lambda_i\right)^2 \\ +\frac{1}{(n-1)(n-2)}\left(\sum_{i=1}^{n-1}\lambda_i\right)^2 \geq \frac{1}{(n-1)(n-2)}\sum_{i=1}^{n-1}\lambda_i^2.$$

Therefore,

$$\left(\lambda_k-\frac{1}{n-1}\sum_{i=1}^{n-1}\lambda_i\right)^2 \geq \frac{1}{(n-1)(n-2)} \\ \times\left[\sum_{i=1}^{n-1}\lambda_i^2-\frac{1}{n-1}\left(\sum_{i=1}^{n-1}\lambda_i\right)^2\right] \geq 0.$$

Since

$$\sum_{i=1}^{n-1} \lambda_i = \sum_{i=1}^{n} \lambda_i = TrL(G) = n,$$

$$\sum_{i=1}^{n-1} \lambda_i^2 = \sum_{i=1}^{n} \lambda_i^2 = \operatorname{Tr} L(G)^2 = n + 2\sum_{u\sim v} \frac{1}{d_u d_v},$$

we can attain

$$\begin{aligned}(\lambda_k - \frac{n}{n-1})^2 &\geq \frac{1}{(n-1)(n-2)}\left(n + 2\sum_{u\sim v}\frac{1}{d_u d_v} - \frac{n^2}{n-1}\right)\\ &= \frac{1}{(n-1)(n-2)}(2\sum_{u\sim v}\frac{1}{d_u d_v} - \frac{n}{n-1}).\end{aligned}$$

By (4) and (5) in Lemma 2.1,

$$\lambda_1 - \frac{n}{n-1} \geq 0, \quad \lambda_{n-1} - \frac{n}{n-1} \leq 0.$$

Hence,

$$\lambda_1 - \frac{n}{n-1} \geq \sqrt{\frac{1}{(n-1)(n-2)}\left(2\sum_{u\sim v}\frac{1}{d_u d_v} - \frac{n}{n-1}\right)},$$

$$\lambda_{n-1} - \frac{n}{n-1} \leq -\sqrt{\frac{1}{(n-1)(n-2)}\left(2\sum_{u\sim v}\frac{1}{d_u d_v} - \frac{n}{n-1}\right)}.$$

So we have

$$\lambda_1 \geq \frac{n}{n-1} + \sqrt{\frac{1}{(n-1)(n-2)}\left(2\sum_{u\sim v}\frac{1}{d_u d_v} - \frac{n}{n-1}\right)}$$

$$\lambda_{n-1} \leq \frac{n}{n-1} - \sqrt{\frac{1}{(n-1)(n-2)}\left(2\sum_{u\sim v}\frac{1}{d_u d_v} - \frac{n}{n-1}\right)}.$$

If the equality in (6) holds, then from the above proof the equality in (8) must hold, so we have $\lambda_1 = \lambda_2 = \cdots = \lambda_{n-1} = n/(n-1)$ and G

must be a complete graph by Lemma 2.1. Conversely, if G is a complete graph, it is easy to see the equality in (6) holds. For the equality in (7), things go in the same way. □

Now we can present the proof of Theorem 1.1.

Proof of Theorem 1.1. By Lemma 2.2 and direct calculation, we can get the result of Theorem 1.1. □

Lemma 2.3 [**11**]. *Let G be a connected graph of order n. Then*

$$\frac{n}{2(n-1)} \leq R_{-1}(G) \leq \left\lfloor \frac{n}{2} \right\rfloor . \tag{9}$$

The left equality holds if and only if G is K_n, and the right equality holds if and only if G is a forest composed of $n/2$ stubs for n even, and a forest composed of $(n-3)/2$ stubs and a $2-$star for n odd.

Lemma 2.4. *Let G be a simple connected graph. If $R_{-1}(G) \leq 1$, then*

$$\lambda_1 < \frac{n}{n-1} + \sqrt{\frac{n-2}{n-1}\left(2R_{-1}(G) - \frac{n}{n-1}\right)}. \tag{10}$$

Proof. Let $M = \sum_{i=1}^{n} \lambda_i^2 = n + 2\sum_{u\sim v}(1/d_u d_v) = n + 2R_{-1}(G)$. We have

$$\lambda_1^2 = M - \sum_{i=2}^{n-1} \lambda_i^2 \leq M - \frac{1}{n-2}\left(\sum_{i=2}^{n-1} \lambda_i\right)^2 = M - \frac{1}{n-2}(n-\lambda_1)^2,$$

namely,

$$\left(1 + \frac{1}{n-2}\right)\lambda_1^2 - \frac{2n}{n-2}\lambda_1 + \frac{n^2}{n-2} - M \leq 0$$
$$(n-1)\lambda_1^2 - 2n\lambda_1 + n^2 - M(n-2) \leq 0.$$

Solving the above inequality, we have

$$\lambda_1 \le \frac{2n + \sqrt{4n^2 - 4(n-1)[n^2 - M(n-2)]}}{2(n-1)} \tag{11}$$
$$= \frac{n}{n-1} + \sqrt{\frac{n-2}{n-1}\left(2R_{-1}(G) - \frac{n}{n-1}\right)}.$$

Note that the normalized Laplacian eigenvalues range from 0 to 2. If $R_{-1}(G) \le 1$, we can get

$$\frac{n}{n-1} + \sqrt{\frac{n-2}{n-1}\left(2R_{-1}(G) - \frac{n}{n-1}\right)} \le 2.$$

If the equality in (11) holds, then from the above proof, we have

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

and so $\lambda_2 = \cdots = \lambda_{n-1}$.

Thus, we have

$$\lambda_1 + (n-2)\lambda_2 = n$$
$$\lambda_1^2 + (n-2)\lambda_2^2 = n + 2R_{-1}.$$

Hence,

$$\lambda_2 = \frac{n}{n-1} + \frac{\sqrt{n[2(n-1)R_{-1}(G) - 1]}}{2(n-1)(n-2)}.$$

We have $\lambda_2 = \lambda_{n-1} > (n/n-1)$; this contradicts Lemma 2.1. So we complete the proof. □

Lemma 2.5 [**12**]. *Let G be a simple graph of order n. Then*

$$R_\alpha(G) \le \frac{1}{2}\rho(G) \sum_{u \in V(G)} d_u^{2\alpha}$$

with equality if G is a regular graph.

Now we can present the proof of Theorem 1.2.

Proof of Theorem 1.2. Since

$$\rho(G) \leq \frac{2}{\sum_{u\in V(G)} d_u^{-2}},$$

namely,

$$\frac{1}{2}\rho(G) \sum_{u\in V(G)} d_u^{-2} \leq 1,$$

by Lemma 2.5, we can get $R_{-1}(G) \leq 1$. Hence, Lemma 2.4 holds. By solving inequality (10), we can get the result. □

Remark. For a connected graph G of order n:

1. If $n \geq 4$ and $\lambda_1 \leq (n+\sqrt{n})/(n-1) \in [0,2]$, then a direct computation shows that

$$\frac{1}{2}(n-1)(n-2)\left(\lambda_1 - \frac{n}{n-1}\right)^2 + \frac{n}{2(n-1)} \leq \frac{n}{2}.$$

So for the upper bound of the Randić index $R_{-1}(G)$, our results (1) in Theorem 1.1 are sometimes better than (9).

2. If $\rho(G) \leq 2/(\sum_{u\in V(G)} d_u^{-2})$, then for the lower bound of the Randić index $R_{-1}(G)$, it is easy to see that (3) in Theorem 1.2 is better than (9).

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