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The Connectivity Index *

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Abstract

Let G be a simple connected graph of order n. The connectivity index $R_\alpha(G)$ of a graph G is the sum of the weights $(d(u)d(v))^\alpha$ of all edges uv of G, where α is a real number ($\alpha \neq 0$), and $d(u)$ denotes the degree of the vertex u. In this paper, we present some new bounds for the connectivity index of a graph G in terms of the eigenvalues of the Laplacian matrix or adjacency matrix of the graph G, from which we can get some known results.

1. Introduction

The connectivity index of an organic molecule whose molecular graph is G is defined (see [5, 12]) as

$$R_\alpha(G) = \sum_{u,v} (d(u)d(v))^\alpha$$

where $d(u)$ denotes the degree of the vertex u of the molecular graph G, where the summation goes over all pairs of adjacent vertices of G and where α ($\alpha \neq 0$) is a pertinently chosen exponent. In 1975, Randić introduced the respective structure-descriptor in [12] for $\alpha = -\frac{1}{2}$ (which he called the *branching index*, and now also called the *Randić index*) in his study of alkanes. The Randić index has been closely correlated with many chemical properties (see [11]). However, other choices of α were also considered, and the exponent α was treated (see [2, 3, 13]) as an adjustable parameter, chosen so as to optimize the correlation between R_α and some selected class of organic compounds. In particular, when ordering isometric alkanes with regard to their connectivity indices one needs to take into account that there exist pairs of isomers whose R_α-values coincide for all α ($\alpha \neq 0$) (see [8]).

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Let $G = (V, E)$ be a simple graph with m edges and vertex set $\{v_1, v_2, \cdots, v_n\}$. For any two vertices $v_i, v_j \in V(G)$ with $i < j$, we will use the symbol $i \sim j$ to denote the edge $v_i v_j$. For $v_i \in V$, the degree of v_i, written by d_i, is the number of edges incident with v_i.

Let $A(G)$ be the adjacency matrix of G and $D(G) = \mathrm{diag}(d_1, d_2, \ldots, d_n)$ be the diagonal matrix of vertex degrees. The Laplacian matrix of G is $L(G) = D(G) - A(G)$. Clearly, $L(G)$ is a real symmetric matrix. From this fact and Geršgorin's Theorem, it follows that its eigenvalues are nonnegative real numbers. The largest eigenvalue of a matrix M is denoted by $\lambda_1(M)$, while for a graph G, we will use $\lambda_i(G)$ to denote $\lambda_i(L(G))$, $i = 1, 2, \ldots, n$ and assume that $\lambda_1(G) \geq \lambda_2(G) \geq \cdots \geq \lambda_{n-1}(G) \geq \lambda_n(G) = 0$. We also use $\rho(G)$ to denote the largest eigenvalue of $A(G)$. When G is connected, $A(G)$ is irreducible and so by Perron-Frobenius Theorem, $\rho(G)$ is simple.

Chemical applications of the eigenvalues of the adjacency matrix are well known and are described in many textbooks and review articles (for a recent review, containing an extensive bibliography, see [4]). Laplacian eigenvalues found chemical applications only relatively recently; for details and further references see [6, 7, 15]. The main chemical applications of Laplacian eigenvalues are in the theory of the Wiener and Kirchhoff indices, and resistance distance [7, 15] and in the theory of photoelectron spectra and ionization potentials of alkanes [6]. So far, no connection between Laplacian eigenvalues and the connectivity index has been reported.

The purpose of this work is to find bounds for the values of $R_\alpha(G)$. These bounds involve the eigenvalues of the Laplacian matrix or adjacency matrix of a graph G.

2. Bounds Involving the Eigenvalues of the Laplacian Matrix

Let G be a simple connected graph and $L(G) = D(G) - A(G)$ be the Laplacian matrix of G. It is well known that $\lambda_n(G) = 0$ with eigenvector $e = (1, 1, \cdots, 1)^T$ and $\lambda_{n-1}(G) > 0$ by G being connected. Since $L(G)$ is symmetric, by the Rayleigh-Ritz Theorem (see for example [10]), we have

$$\lambda_{n-1}(G) = \inf_{x \perp e, x \neq 0} \frac{x^T L(G) x}{x^T x} \tag{1}$$

and

$$\lambda_1(G) = \sup_{x \neq 0} \frac{x^T L(G) x}{x^T x}. \tag{2}$$

Now we introduce the graph invariant k as

$$k = \sum_{i=1}^{n} d_i^{2\alpha} - \frac{\left(\sum_{i=1}^{n} d_i^{\alpha}\right)^2}{n}. \tag{3}$$

By the Cauchy-Schwarz inequality, $k \geq 0$ and $k = 0$ if and only if $d_i = d_j$ for $1 \leq i, j \leq n$.

Theorem 1. *Let G be a simple connected graph of order n. Then*

$$\frac{1}{2} \sum_{i=1}^{n} d_i^{2\alpha+1} - \frac{k}{2} \lambda_1(G) \leq R_\alpha(G) \leq \frac{1}{2} \sum_{i=1}^{n} d_i^{2\alpha+1} - \frac{k}{2} \lambda_{n-1}(G). \tag{4}$$

where k is the graph invariant. Moreover, $R_\alpha(G) = \frac{1}{2} \sum_{i=1}^{n} d_i^{2\alpha+1}$ (and $k = 0$) if and only if G is a regular graph.

Proof. If G is an s-regular graph of order n, then $R_\alpha(G) = \frac{n}{2}s^{2\alpha+1}$ and $k = 0$ by an elementary calculation. Therefore the inequalities (4) hold. Conversely, if $R_\alpha(G) = \frac{1}{2}\sum_{i=1}^{n} d_i^{2\alpha+1}$, then $k = 0$ and thus G is a regular graph obviously.

So in the following we assume that G is not regular.

Set $d = (d_1^\alpha, d_2^\alpha, \cdots, d_n^\alpha)^T$ and $\theta = -\frac{\sum_{i=1}^{n} d_i^\alpha}{n}$. Denote $x = \theta e + d$. Then $x \neq 0$ by G being not regular and $x \perp e$. A simple calculation shows that $x^T x = k > 0$. On the other hand, since $L(G)e = 0$, $x^T L(G) x = d^T L(G) d$. Note that

$$\begin{aligned} d^T L(G) d &= d^T (D - A) d = \sum_{i=1}^{n} d_i^{2\alpha+1} - 2\sum_{i\sim j} d_i^\alpha d_j^\alpha \\ &= \sum_{i=1}^{n} d_i^{2\alpha+1} - 2R_\alpha(G), \end{aligned}$$

where $i \sim j$ runs over all the edges of G. Thus by (1) and (2), we have

$$\lambda_{n-1}(G) \leq \frac{x^T L(G) x}{x^T x} \leq \lambda_1(G)$$

and (4) follows immediately. ∎

Since $k = \sum_{i=1}^{n} d_i^{2\alpha} - \frac{\left(\sum_{i=1}^{n} d_i^\alpha\right)^2}{n} \geq 0$ and $\lambda_{n-1}(G) > 0$ if G is connected, we have the following two corollaries.

Corollary 2. *Let G be a simple connected graph of order n and α be a real number with $\alpha \neq 0$. Then*

$$R_\alpha(G) \leq \frac{1}{2}\sum_{i=1}^{n} d_i^{2\alpha+1}$$

with equality if and only if G is a regular graph.

Corollary 3. *Let G be a simple connected graph of order n. Then*

$$R_{-\frac{1}{2}}(G) \leq \frac{n}{2}$$

with equality if and only if G is a regular graph.

Corollary 4. *Let G be a simple non-regular graph of order n and α be a real number with $\alpha \neq 0$. Then*

$$R_\alpha(G) \geq \frac{1}{2}\left(\sum_{i=1}^{n} d_i^{2\alpha+1} + \left(\sum_{i=1}^{n} d_i^\alpha\right)^2 - n\sum_{i=1}^{n} d_i^{2\alpha}\right)$$

with equality if G is the star.

Proof. Since $\lambda_1 \leq n$, by Theorem 1, we have $R_\alpha(G) \geq \frac{1}{2}\sum_{i=1}^{n} d_i^{2\alpha+1} - \frac{1}{2}kn$. Thus

$$R_\alpha(G) \geq \frac{1}{2}\left(\sum_{i=1}^{n} d_i^{2\alpha+1} + \left(\sum_{i=1}^{n} d_i^\alpha\right)^2 - n\sum_{i=1}^{n} d_i^{2\alpha}\right).$$

If $G = K_{1,n-1}$, then we can assume that $d_1 = n - 1$, $d_2 = \cdots = d_n = 1$. Hence

$$\sum_{i=1}^{n} d_i^{2\alpha+1} + \left(\sum_{i=1}^{n} d_i^\alpha\right)^2 - n\sum_{i=1}^{n} d_i^{2\alpha}$$

$$= (n - 1 + (n-1)^{2\alpha+1}) + (n - 1 + (n-1)^{\alpha})^2 - n(n - 1 + (n-1)^{2\alpha})$$
$$= 2(n-1)^{\alpha+1} = 2R_\alpha(G).$$

■

3. Bounds Involving the Eigenvalues of the Adjacency Matrix

Let $A(G)$ be the adjacency matrix of graph G and $\rho(G)$ the largest eigenvalue of $A(G)$.

Theorem 5. *Let G be a simple graph of order n. Then*

$$R_\alpha(G) \leq \frac{1}{2}\rho(G)\sum_{i=1}^{n} d_i^{2\alpha} \tag{5}$$

with equality if G is a regular graph.

Proof. Note that $A(G)$ is symmetric. By the Rayleigh-Ritz Theorem (see for example [10]), we have

$$\rho(G) = \sup_{x \neq 0} \frac{x^T A(G) x}{x^T x}. \tag{6}$$

Set $y = (d_1^\alpha, d_2^\alpha, \cdots, d_n^\alpha)^T$. Then

$$y^T y = \sum_{i=1}^{n} d_i^{2\alpha}$$

and

$$y^T A(G) y = 2R_\alpha(G).$$

Thus by (6), we have

$$R_\alpha(G) \leq \frac{1}{2}\rho(G)\sum_{i=1}^{n} d_i^{2\alpha}.$$

If G is an s-regular graph, then $R_\alpha(G) = \frac{n}{2}s^{2\alpha+1}$ by an elementary calculation. On the other hand, $\rho(G) = s$ if G is s-regular. Thus the equality (5) holds. ■

In [9], Hofmeister showed that $\rho(G) \geq \sqrt{\frac{1}{n}\sum_{i=1}^{n} {d_i}^2}$, with equality if and only if G is either a regular connected graph or a semiregular connected bipartite graph. Therefore we have

$$\sum_{i=1}^{n} d_i^2 \leq n\rho^2(G). \tag{7}$$

By Theorem 5 and (7), we have the following corollary:

Corollary 6. *Let G be a simple graph of order n. Then*

$$R_1(G) \leq \frac{n}{2}\rho^3(G). \tag{8}$$

with equality if G is a regular connected graph.

Remark 7. For a graph $G = (V, E)$ with size m, Bollobás and Erdős [1] prove that

$$R_1(G) \leq m\left(\frac{\sqrt{8m+1} - 1}{2}\right)^2 \tag{9}$$

The bounds (8) and (9) are incomparable: for example, when $G \cong K_{\frac{n}{2},\frac{n}{2}}$, the upper bound (8) is $n^4/16$ and better than (9); however, when $G \cong K_{1,n-1}$, $n \geq 10$, the upper bound (9) is better than (8).

Let G be a graph with n vertices and m edges. Denote

$$b(\alpha) = 2^{-\alpha} n^{\alpha} m^{1-\alpha}.$$

Obviously, $b(\alpha)b(-\alpha) = m^2$. Then Corollary 6 can be generalized to the following result.

Theorem 8. *Let $G = (V, E)$ be a graph with n vertices and m edges. Then*

$$R_\alpha(G) \geq b(\alpha)\rho^{3\alpha}(G)$$

for $-1 \leq \alpha < 0$, and

$$R_\alpha(G) \leq b(\alpha)\rho^{3\alpha}(G)$$

for $0 < \alpha \leq 1$.

Proof. For $\alpha = 1$, the result follows by Corollary 6. Therefore in the following proof, we may assume that $\alpha \neq 1$. Suppose first that $0 < \alpha < 1$ and set $\beta = 1 - \alpha$, $s = 1/\alpha$, $t = 1/\beta$. Then $1/s + 1/t = 1$. By Hölder's inequality and Corollary 6, we have

$$\begin{aligned} R_\alpha(G) &= \sum_{i\sim j}(d_i d_j)^\alpha \cdot 1^\beta \\ &\leq \left(\sum_{i\sim j}(d_i d_j)^{\alpha s}\right)^{1/s} \left(\sum_{i\sim j} 1\right)^{1/t} \\ &= R_1^\alpha(G) m^\beta \leq b(\alpha)\rho^{3\alpha}(G). \end{aligned}$$

On the other hand, by the Cauchy-Schwartz inequality, for $\alpha \neq 0$, we have

$$\begin{aligned} m &= \sum_{i\sim j}(d_i d_j)^{\alpha/2}(d_i d_j)^{-\alpha/2} \\ &\leq \left(\sum_{i\sim j}(d_i d_j)^\alpha\right)^{1/2} \left(\sum_{i\sim j}(d_i d_j)^{-\alpha}\right)^{1/2} \\ &= R_\alpha^{1/2}(G) R_{-\alpha}^{1/2}(G). \end{aligned}$$

That is,

$$R_\alpha(G) R_{-\alpha}(G) \geq m^2.$$

Therefore, if $-1 \leq \alpha < 0$, then

$$R_\alpha(G) \geq \frac{m^2}{R_{-\alpha}(G)} \geq \frac{b(\alpha)b(-\alpha)}{b(-\alpha)\rho^{-3\alpha}(G)} = b(\alpha)\rho^{3\alpha}(G).$$

■

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