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The m-connectivity index of graphs *

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Abstract

The m-connectivity index ${}^m\chi_\alpha(G)$ of an organic molecule whose molecular graph is G is the sum of the weights $(d_{i_1}d_{i_2}...d_{i_{m+1}})^\alpha$, where $i_1 - i_2 - ... - i_{m+1}$ runs over all paths of length m in G and d_i denotes the degree of vertex v_i. We find upper bounds for ${}^m\chi_\alpha(G)$ when $m \geq 1$ and $\alpha \geq -1$ $(\alpha \neq 0)$ using the eigenvalues of the Laplacian matrix of an associated weighted graph.

1 Introduction

The connectivity index of an organic molecule whose molecular graph is G is defined (see [4] [11]) as

$$ {}^1\chi_\alpha(G) = \sum_{u,v}(d(u)d(v))^\alpha $$

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 [11] for $\alpha = -\frac{1}{2}$ (which he called the *branching index*, and is now also called the *Randić index*) in his study of alkanes. The Randić index has been closely correlated with many chemical properties (see [7]). 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 ${}^1\chi_\alpha$ and some selected class of organic compounds. In particular, when ordering isomeric alkanes with regard to their connectivity indices one needs to take into account that there exist pairs of isomers whose ${}^1\chi_\alpha$-values coincide for all α $(\alpha \neq 0)$ (see [5]).

Let $G = (V, E)$ be a simple graph with 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 $i - j$ to denote the edge v_iv_j. For $v_i \in V$, the degree of v_i, written by d_i, is the number of edges incident with v_i.

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For an integer $m \geq 1$, the m-connectivity index is defined as

$$^{m}\chi_{\alpha}(G) = \sum_{i_1 - i_2 - \cdots - i_{m+1}} (d_{i_1} d_{i_2} \cdots d_{i_{m+1}})^{\alpha}$$

where $i_1 - i_2 - \cdots - i_{m+1}$ runs over all paths (that is, $i_s \neq i_t$ for $1 \leq s < t \leq m+1$) of length m of G.

The higher connectivity indices are of great interest in molecular graph theory ([8], [14]) and some of their mathematical properties have been reported in [1], [10] and [12].

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 $\lambda_1(G) \geq \lambda_2(G) \geq \cdots \geq \lambda_{n-1}(G) \geq \lambda_n(G) = 0$.

The purpose of this work is to find upper bounds for the values of m-connectivity index of a graph.

2 The 1-connectivity index of weighted graphs

Let $G = (V, E, \omega)$ be a weighted simple graph which has assigned a certain weight $\omega(i,j)$ for each pair v_i, v_j of vertices. The weights are usually non-negativity real numbers and they must satisfy the following conditions:

(1) $\omega(i,j) = \omega(j,i)$, $v_i, v_j \in V(G, \omega)$, and

(2) $\omega(i,j) \neq 0$, if and only if v_i and v_j are adjacent in (G, ω).

Let ω_i denote the degree of $v_i \in V(G, \omega)$, that is, $\omega_i = \sum_j \omega(i,j)$. We call (G, ω) a s-regular weighted graph if $\omega_i = s$ for $1 \leq i \leq n$. The Laplacian matrix $L(G, \omega)$ of (G, ω) is a $n \times n$ matrix with entries

$$L_{i,j} = \begin{cases} \omega_i & \text{if } i = j \\ -\omega(i,j) & \text{if } i - j \\ 0 & \text{else.} \end{cases}$$

Then $L(G, \omega)$ is still a real symmetric matrix and

$$x^T L(G, \omega) x = \sum_{i-j} \omega(i,j)(x_i - x_j)^2,$$

where x is a vector. From this fact and Geršgorin's Theorem, it follows that its eigenvalues are nonnegative real numbers and they will also be denoted by $\lambda_1(G, \omega) \geq \cdots \geq \lambda_{n-1}(G, \omega) \geq \lambda_n(G, \omega) \geq 0$. Obviously, $\lambda_n(G, \omega) = 0$ and a corresponding eigenvector is $e = (1, 1, \cdots, 1)^T$.

Since $L(G,\omega)$ is symmetric, by the Rayleigh-Ritz Theorem (see for example [6]), we have

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

and

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

The m-connectivity index of the weighted graph (G,ω) is defined as

$$^m\chi_\alpha(G,\omega) = \sum_{i_1-i_2-\cdots-i_{m+1}} \omega(i_1,i_2)\cdots\omega(i_m,i_{m+1})(\omega_{i_1}\omega_{i_2}\cdots\omega_{i_{m+1}})^\alpha$$

where $i_1 - i_2 - \cdots - i_{m+1}$ runs over all paths of length m of (G,ω).

Now we introduce the graph invariant k as

$$k = \sum_{i=1}^n \omega_i^{2\alpha} - \frac{(\sum_{i=1}^n \omega_i^\alpha)^2}{n}.$$

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

In full analogy to a result earlier proven in [9] for non-weighted graphs, we have the following result.

Theorem 2.1. *Let $G = (V,E,\omega)$ be a weighted simple graph. Then*

$$\frac{1}{2}\sum_{i=1}^n \omega_i^{2\alpha+1} - \frac{\kappa}{2}\lambda_1(G,\omega) \leq {}^1\chi_\alpha(G,\omega) \leq \frac{1}{2}\sum_{i=1}^n \omega_i^{2\alpha+1} - \frac{\kappa}{2}\lambda_{n-1}(G,\omega), \tag{3}$$

where κ is a graph invariant defined as above. Moreover ${}^1\chi_\alpha(G,\omega) = \frac{1}{2}\sum_{i=1}^n \omega_i^{2\alpha+1}(\kappa = 0)$, if and only if (G,ω) is regular.

Let G be a simple graph with n vertices. We assign a certain weight $\omega(i,j)$ to the edge of G such that $\omega(i,j) = 1$ for all $i - j$. Then $d_i = \omega_i$ for $i = 1,2,\cdots,n$. Thus by Theorem 2.1, we obtain the following result.

Theorem 2.2 [9]. *Let G be a simple graph with vertices $v_1, v_2, \cdots, v_n$. Then*

$$\frac{1}{2}\sum_{i=1}^n d_i^{2\alpha+1} - \frac{\kappa}{2}\lambda_1(G) \leq {}^1\chi_\alpha(G) \leq \frac{1}{2}\sum_{i=1}^n d_i^{2\alpha+1} - \frac{\kappa}{2}\lambda_{n-1}(G),$$

where κ is a graph invariant defined as $\kappa = \sum_{i=1}^n d_i^{2\alpha} - \frac{(\sum_{i=1}^n d_i^\alpha)^2}{n}$. Moreover ${}^1\chi_\alpha(G) = \frac{1}{2}\sum_{i=1}^n d_i^{2\alpha+1}(\kappa = 0)$, if and only if G is regular.

3 Upper bounds for m-connectivity index of simple graphs

In this section, we will consider m-connectivity index of a graph for $m \geq 1$ and $\alpha \geq -1$, $\alpha \neq 0$. The idea of the construction of the following weighted graph comes from [1].

(1) Let G be a simple graph with vertices $v_1, v_2, \cdots, v_n$ $(n = |V(G)|)$ and d_i be the degree of v_i. We assume that every connected component of G has at least two vertices. We want to find bounds for ${}^m\chi_\alpha(G)$, $m \geq 1$. For $m \geq 1$, we introduce a weighted graph $G^{(m)} = (V^{(m)}, E^{(m)}, \omega^{(m)})$ in the following way: the vertices of $G^{(m)}$ are those of the vertices in G; there is an edge $i - j$ in $G^{(m)}$ if there is a path $i = i_1 - i_2 - \cdots - i_{m+1} = j$ in G; $\omega^{(1)}(i,j) = 1$ and

$$\omega^{(m)}(i,j) = \sum_{i=i_1-i_2-\ldots-i_{m+1}=j} (d_{i_2}\ldots d_{i_m})^\alpha \qquad m \geq 2,$$

where the sum runs over all paths in G of length m between i and j. Obviously $|V(G^{(m)})| = n$. Let $\omega_i^{(m)}$ be the degree of a vertex v_i in the weighted graph $G^{(m)}$, that is,

$$\omega_i^{(m)} = \sum_{v_iv_j \in E^{(m)}} \omega^{(m)}(i,j).$$

Then we have the following lemma.

Lemma 3.1. *For $1 \leq i \leq n$ and $\alpha \geq -1$ $(\alpha \neq 0)$, we have*

$$\delta^{m-1} d_i \leq \omega_i^{(m)} \leq \triangle^{m-1} d_i, \tag{4}$$

where $\Delta = (d_{\max} - 1)d_{\max}^\alpha$ for $d_{\max} = \max\{d_i : 1 \leq i \leq n\}$ and $\delta = (d_{\min} - 1)d_{\min}^\alpha$ for $d_{\min} = \min\{d_i : 2 \leq d_i\}$.

Proof. If $m = 1$, then $G^{(m)} = G$, $\omega_i^{(1)} = d_i$ and (4) holds obviously. So we may assume that $m \geq 2$. By definition,

$$\begin{aligned}
\omega_i^{(m)} &= \sum_{v_iv_j \in E^{(m)}} \omega^{(m)}(i,j) = \sum_j \sum_{i=i_1-i_2-\ldots-i_{m+1}=j} (d_{i_2}\ldots d_{i_m})^\alpha \\
&= \sum_{i_m} \sum_{i=i_1-i_2-\ldots-i_m} (d_{i_2}\ldots d_{i_{m-1}})^\alpha d_{i_m}^\alpha (d_{i_m} - 1),
\end{aligned}$$

the last equality due to the fact that there are $d_{i_m} - 1$ choices for $v_j = v_{i_{m+1}}$ once the path $i = i_1 - i_2 - \ldots - i_m$ is fixed. Obviously, $d_{i_j} \geq 2$ for $2 \leq j \leq m$. Since $\delta \leq d_x^\alpha(d_x - 1) \leq \Delta$ for any vertices with $d_x \geq 2$ and $\alpha \geq -1$, then

$$\delta\omega_i^{(m-1)} \leq \omega_i^{(m)} \leq \omega_i^{(m-1)}\Delta$$

and the result follows by induction. ■

(2) The connectivity index ${}^1\chi_\alpha(G^{(m)}, \omega^{(m)})$ of the weighted graph $G^{(m)} = (V^{(m)}, E^{(m)}, \omega^{(m)})$ and the m-connectivity index ${}^m\chi_\alpha(G)$ of G are related in the following simple way.

Lemma 3.2.

$${}^m\chi_\alpha(G)\delta^{2\alpha(m-1)} \leq {}^1\chi_\alpha(G^{(m)}, \omega^{(m)}) \leq {}^m\chi_\alpha(G)\Delta^{2\alpha(m-1)}, \quad \alpha > 0; \tag{5}$$

$${}^m\chi_\alpha(G)\Delta^{2\alpha(m-1)} \leq {}^1\chi_\alpha(G^{(m)}, \omega^{(m)}) \leq {}^m\chi_\alpha(G)\delta^{2\alpha(m-1)}, \quad -1 \leq \alpha < 0. \tag{6}$$

Proof. By definition

$$\begin{aligned} {}^1\chi_\alpha(G^{(m)},\omega^{(m)}) &= \sum_{i-j}\omega^{(m)}(i,j)(\omega_i^{(m)}\omega_j^{(m)})^\alpha \\ &= \sum_{i=i_1-i_2-\ldots-i_{m+1}=j}\left[\frac{\omega_i^{(m)}\omega_j^{(m)}}{d_i d_j}\right]^\alpha (d_{i_1}d_{i_2}\ldots d_{i_m}d_{i_{m+1}})^\alpha \end{aligned}$$

where the last sum runs over all paths $i = i_1 - i_2 - \ldots - i_{m+1} = j$ of length m in G. The inequalities follow from Lemma 3.1. ∎

The following is the main result of the paper.

Theorem 3.3. *Let G be a simple graph with vertices $v_1, v_2, \cdots, v_n$. Let $d_{\max}$ be the maximal value of d_i $(1 \le i \le n)$, $\triangle = (d_{\max}-1)d_{\max}^\alpha$, $d_{\min} = \min\{d_i : 2 \le d_i\}$ and $\delta = (d_{\min}-1)d_{\min}^\alpha$. Then*

$$ {}^m\chi_\alpha(G) \le \frac{\Delta^{(m-1)(2\alpha+1)}}{2\delta^{2\alpha(m-1)}}\sum_{i=1}^n d_i^{2\alpha+1} \qquad \alpha > 0, \tag{7}$$

$$ {}^m\chi_\alpha(G) \le \frac{\Delta^{m-1}}{2}\sum_{i=1}^n d_i^{2\alpha+1} \qquad -\frac{1}{2} \le \alpha < 0. \tag{8}$$

and

$$ {}^m\chi_\alpha(G) \le \frac{\delta^{(m-1)(2\alpha+1)}}{2\Delta^{2\alpha(m-1)}}\sum_{i=1}^n d_i^{2\alpha+1} \qquad -1 \le \alpha \le -\frac{1}{2}. \tag{9}$$

Proof. We define $G^{(m)} = (V^{(m)}, E^{(m)}, \omega^{(m)})$ as above. By (3), we have

$$\begin{aligned} {}^1\chi_\alpha(G^{(m)},\omega^{(m)}) &\le \frac{1}{2}\sum_{i=1}^n(\omega_i^{(m)})^{2\alpha+1} - \frac{\kappa}{2}\lambda_{n-1}(G^{(m)},\omega^{(m)}) \\ &\le \frac{1}{2}\sum_{i=1}^n(\omega_i^{(m)})^{2\alpha+1}. \end{aligned}$$

If $\alpha > 0$, then by Lemmas 3.1 and 3.2, we have that

$$\begin{aligned} {}^m\chi_\alpha(G) &\le \frac{1}{\delta^{2\alpha(m-1)}}({}^1\chi_\alpha(G^{(m)},\omega^{(m)})) \\ &\le \frac{1}{2\delta^{2\alpha(m-1)}}\sum_{i=1}^n(\omega_i^{(m)})^{2\alpha+1} \\ &\le \frac{\Delta^{(m-1)(2\alpha+1)}}{2\delta^{2\alpha(m-1)}}\sum_{i=1}^n d_i^{2\alpha+1}. \end{aligned}$$

If $-\frac{1}{2} \le \alpha < 0$, then $2\alpha+1 \ge 0$. Thus, by Lemmas 3.1 and 3.2, we have that

$$\begin{aligned} {}^m\chi_\alpha(G) &\le \frac{1}{\Delta^{2\alpha(m-1)}}({}^1\chi_\alpha(G^{(m)},\omega^{(m)})) \\ &\le \frac{1}{2\Delta^{2\alpha(m-1)}}\sum_{i=1}^n(\omega_i^{(m)})^{2\alpha+1} \\ &\le \frac{\Delta^{m-1}}{2}\sum_{i=1}^n d_i^{2\alpha+1}. \end{aligned}$$

If $-1 \leq \alpha \leq -\frac{1}{2}$, then $2\alpha + 1 \leq 0$. Thus by Lemmas 3.1 and 3.2, we have that

$$\begin{aligned} {}^m\chi_\alpha(G) &\leq \frac{1}{\Delta^{2\alpha(m-1)}}({}^1\chi_\alpha(G^{(m)}, \omega^{(m)})) \\ &\leq \frac{1}{2\Delta^{2\alpha(m-1)}}\sum_{i=1}^{n}(\omega_i^{(m)})^{2\alpha+1} \\ &\leq \frac{\delta^{(m-1)(2\alpha+1)}}{2\Delta^{2\alpha(m-1)}}\sum_{i=1}^{n} d_i^{2\alpha+1}. \end{aligned}$$

■

In particular, if $\alpha = -\frac{1}{2}$, then we have the following corollary by Theorem 3.3.

Corollary 3.4. [1] *Let G be a simple graph with vertices $v_1, v_2, \cdots, v_n$. Let d_{max} be the maximal value of d_i $(1 \leq i \leq n)$ and $\Delta' = (d_{max} - 1)/\sqrt{d_{max}}$. Then*

$${}^m\chi_{-\frac{1}{2}}(G) \leq \frac{n(\Delta')^{m-1}}{2}.$$

If $m = 1$, then we have the following corollary by Theorem 3.3.

Corollary 3.5. *Let G be a simple graph with vertices $v_1, v_2, \cdots, v_n$. Then*

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

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References

[1] O. Araujo and J.A. de la Peña, The connectivity index of a weighted graph, Lin. Alg. Appl. 283(1998) 171-177.

[2] E. Estrada, Graph theoretical invariant of Randic revisited, J. Chem. Inf. Comput. Sci. 35(1995) 1022-1025.

[3] E. Estrada, Connectivity polynomial and long-range contributions in the molecular connectivity model, Chem. Phys. Lett. 312(1999), 556-560.

[4] I. Gutman and M. Lepović, Choosing the exponent in the definition of the connectivity, J. Serb. Chem. Soc. 66(2001) 605-611.

[5] I. Gutman, D. Vidović and A. Nedić, Ordering of alkane isomers by means of connectivity indices, J. Serb. Chem. Soc. 67(2)(2002) 87-97.

[6] R.A. Horn, C.R. Johnson, Matrix Analysis, Cambridge Univ. Press, Cambridge, 1985.

[7] L.B. Kier and L.H. Hall, Molecular Connectivity in Chemistry and Drug Research, Academic Press, San Francisco, 1976.

[8] L.B. Kier, W.J. Murray, M. Randić and L.H. Hall, Molecular connectivity V: connectivity series concept applied to density, J. Pharm. Sci. 65(1976) 1226-1230.

[9] M. Lu, H. Liu and F. Tian, The connectivity index, MATCH Commun. Math. Comput. Chem. 51(2004) 149-154.

[10] J. Rada and O. Araujo, Higher order connectivity index of starlike trees, Discr. Appl. Math. 119(2002) 287-295.

[11] M. Randić, On characterization of molecular branching, J. Amer. Chem. Soc. 97(1975) 6609-6615.

[12] M. Randić, Representation of molecular graphs by basic graphs, J. Chem. Inf. Comput. Sci. 32(1992) 57-69.

[13] M. Randić, P.J. Hansen and P.C. Jurs, Search for useful graph theoretical invariants of molecular structure, J. Chem. Inf. Comput. Sci. 28(1988) 60-68.

[14] V.K. Singh, V.P. Tewary, D.K. Gupta and A.K. Srivastava, Calculation of heat of formation: molecular connectivity and IOC-ω technicque, a comparative study, Tetrahedron 40(1984) 2859-2863.