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Estimating the higher-order Randić index

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ABSTRACT

Let G be a (molecular) graph with vertex set $V = \{v_1, v_2, \ldots, v_n\}$. Let $\delta(v_i)$ be the degree of the vertex $v_i \in V$. If the vertices $v_{i_1}, v_{i_2}, \ldots, v_{i_{h+1}}$ form a path of length $h, h \geqslant 1$, in the graph G, then the hth order Randić index R_h of G is defined as the sum of the terms $1/\sqrt{\delta(v_{i_1})\delta(v_{i_2}), \ldots, \delta(v_{i_{h+1}})}$ over all paths of length h contained (as subgraphs) in G. Lower and upper bounds for R_h are obtained, in terms of the vertex degree sequence of G. Closed formulas for R_h are obtained for the case when G is regular or semiregular bipartite.

1. Introduction

In this Letter we consider simple graphs $G = (V, E)$ with n vertices and m edges. Let $V = \{v_1, v_2, \ldots, v_n\}$ be the vertex set of G, and let $\delta_i = \delta(v_i)$ denote the degree of the vertex v_i. Without loss of generality we may assume that $\delta_1 \geqslant \delta_2 \geqslant \cdots \geqslant \delta_n$. The maximum and minimum vertex degree will be denoted by Δ and δ, respectively. In other words, $\delta_1 = \Delta$ and $\delta_n = \delta$. In chemical applications it is usually $\delta = 1$ (e.g., in the molecular graphs of alkanes) or $\delta = 2$ (e.g., in the molecular graphs of benzenoid hydrocarbons); in molecular graphs it is always $\Delta \leqslant 4$ [1].

The *Randić index* $R_1(G)$ of a graph G was introduced in 1975 [2] and defined as

$$R_1 = R_1(G) = \sum_{v_i, v_j \in E} \frac{1}{\sqrt{\delta(v_i)\delta(v_j)}} \tag{1}$$

This graph invariant, sometimes referred to as *connectivity index*, has been successfully related to a variety of physical, chemical, and pharmacological properties of organic molecules and became one of the most popular molecular-structure descriptors [2–6]. After the publication of the seminal paper [7], mathematical properties of R_1 were extensively studied, see [7–10] and the references cited therein.

The *higher-order Randić indices* are also of interest in chemical graph theory [3,4,11,12]. For $h \geqslant 1$, the hth order Randić index $R_h(G)$ of a graph G is defined as

$$R_h = R_h(G) = \sum_{v_{i_1} v_{i_2} \ldots, v_{i_{h+1}} \in \mathscr{P}_h} \frac{1}{\sqrt{\delta(v_{i_1})\delta(v_{i_2}) \cdots \delta(v_{i_{h+1}})}} \tag{2}$$

where $\mathscr{P}_h$ denotes the set of paths of length h contained (as subgraphs) in G.

Of the higher-order Randić indices the most frequently applied is R_2; for more details see [3,5,13,14].

So far only a few mathematical results have been published on this class of graph invariants [13–19]. We point out two results as examples. The following upper bound was obtained in [15] by Araujo and de la Peña,

$$R_h \leqslant \frac{n_h + c_h}{2} \left(\frac{\Delta - 1}{\sqrt{\Delta}} \right)^{h-1} \tag{3}$$

where n_h is the number of vertices v in G, such that there is at least one path of length h starting at v, and c_h is the number of vertices v which accept a path of length h from v to v.

The *weighted adjacency matrix* of a graph G of order n, was introduced by the second author of this Letter [13,20] as the $n \times n$ matrix $\mathscr{A}$ whose (i,j)-entry is

$$a_{ij} = \begin{cases} \frac{1}{\sqrt{\delta(v_i)\delta(v_j)}}, & v_i \sim v_j \\ 0 & \text{otherwise} \end{cases} \tag{4}$$

where by $v_i \sim v_j$ is indicated that the vertices v_i and v_j are adjacent. This matrix was used in the study of the Randić index and conditional parameters in graphs [20] and elsewhere [21]. Moreover, if $\lambda_1, \lambda_2, \ldots, \lambda_n$ are the eigenvalues of $\mathscr{A}$, then there is a following relation between R_2 and R_1 [13]:

$$R_2 \geqslant \left(\frac{(2R_1 - \phi)^2}{n - \phi} + \phi - \tau \right) \frac{\sqrt{\delta}}{2} \tag{5}$$

where

$$\tau = \sum_{i=1}^{n} \lambda_i^2 \quad \text{and} \quad \phi = \frac{1}{2m} \left(\sum_{v \in V} \sqrt{\delta(v)} \right)^2 \tag{6}$$

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The purpose of this note is to find bounds for R_h in terms of the degree sequence of G. As a consequence, we obtain closed formulas for the case of regular graphs and semiregular bipartite graphs.

Recall that a graph is said to be regular (of degree r) if all its vertices have equal degrees (equal to r); for instance, the molecular graphs of fullerenes are regular of degree 3. A bipartite graph is said to be semiregular (of degrees r', r'') if for any two adjacent vertices u, v it holds $\delta(u) = r'$ and $\delta(v) = rq''$.

2. Results

The *girth* of a graph is the size of its smallest cycle. For instance, the molecular graphs of benzenoid hydrocarbons have girth 6. The molecular graphs of biphenylene and azulene have girth 4 and 5, respectively [1].

Theorem 1. *Let $G = (V, E)$ be a graph with girth $g(G)$ and degree sequence $\delta_1 \geqslant \delta_2 \geqslant \cdots \geqslant \delta_n$, $\delta_1 = \Delta$, $\delta_n = \delta$. If $\delta \geqslant 2$ and $g(G) > h$, then*

$$\frac{(\delta-1)^{h-2}}{2\sqrt{\Delta^h}}\sum_{i=1}^{n}(\delta_i-1)\sqrt{\delta_i} \leqslant R_h(G) \leqslant \frac{(\Delta-1)^{h-2}}{2\sqrt{\delta^h}}\sum_{i=1}^{n}(\delta_i-1)\sqrt{\delta_i} \quad (7)$$

Proof. Since $\delta \geqslant 2$, for every $v \in V$, the number of paths of length 2 in G of the form $v_i v v_j$ is $\delta(v)(\delta(v)-1)/2$. So, we have

$$R_2 = \sum_{v_i v_j v_k \in \mathscr{P}_2} \frac{1}{\sqrt{\delta(v_i)\delta(v_j)\delta(v_k)}} \geqslant \sum_{j=1}^{n} \frac{\delta(v_j)(\delta(v_j)-1)}{2} \frac{1}{\sqrt{\Delta\delta(v_j)\Delta}} \quad (8)$$

and

$$R_2 = \sum_{v_i v_j v_k \in \mathscr{P}_2} \frac{1}{\sqrt{\delta(v_i)\delta(v_j)\delta(v_k)}} \leqslant \sum_{j=1}^{n} \frac{\delta(v_j)(\delta(v_j)-1)}{2} \frac{1}{\sqrt{\delta\delta(v_j)\delta}} \quad (9)$$

Therefore, the result follows for $h = 2$.

Suppose now that $h \geqslant 3$. Given a vertex $u \in V$, let $\mathscr{P}_h(u)$ be the set of paths of length h whose second vertex is u, that is, paths of the form $u_1 u u_2, \ldots, u_h$. We denote by $N(v)$ the set of neighbors of an arbitrary vertex $v \in V$. Note that the degree of v is $\delta(v) = |N(v)|$. If $\delta \geqslant 2$, then for every $v \in V$ and $w \in N(v)$ we have $N(w)\setminus\{v\} \neq \emptyset$. So, for every $u \in V$, there exists a vertex sequence $u_1 u u_2, \ldots, u_h$ such that $u_1, u_2 \in N(u)$, $u_3 \in N(u_2)\setminus\{u\}$, $u_4 \in N(u_3)\setminus\{u_2\}, \ldots$, $u_h \in N(u_{h-1})\setminus\{u_{h-2}\}$. If $g(G) > h$, then the sequence $u_1 u u_2, \ldots, u_h$ is a path. Conversely, every path of length h whose second vertex is u can be constructed as above. Hence, the number of paths of length h whose second vertex is u is bounded by

$$|\mathscr{P}_h(u)| \geqslant \min_{u_1 u u_2,\ldots,u_h \in \mathscr{P}_h(u)} \left\{\delta(u)(\delta(u)-1)\prod_{j=2}^{h-1}(\delta(u_j)-1)\right\} \geqslant \delta(u)(\delta(u)-1)(\delta-1)^{h-2} \quad (10)$$

and

$$|\mathscr{P}_h(u)| \leqslant \max_{u_1 u u_2,\ldots,u_h \in \mathscr{P}_h(u)} \left\{\delta(u)(\delta(u)-1)\prod_{j=2}^{h-1}(\delta(u_j)-1)\right\} \leqslant \delta(u)(\delta(u)-1)(\Delta-1)^{h-2}. \quad (11)$$

On the other hand, the higher-order Randić index of G is bounded by

$$\frac{1}{2}\sum_{u\in V}|\mathscr{P}_h(u)|\frac{1}{\sqrt{\delta(u)}\sqrt{\Delta^h}} \leqslant R_h \leqslant \frac{1}{2}\sum_{u\in V}|\mathscr{P}_h(u)|\frac{1}{\sqrt{\delta(u)}\sqrt{\delta^h}} \quad (12)$$

Thus, by (10)–(12) we deduce the bounds stated in Theorem 1. □

Corollary 2. *Let $G = (V, E)$ be a graph of girth $g(G)$, order n, size m, minimum degree δ and maximum degree Δ. If $\delta \geqslant 2$ and $g(G) > h$, then*

$$\frac{(2m-n)(\delta-1)^{h-2}}{2}\sqrt{\frac{\delta}{\Delta^h}} \leqslant R_h(G) \leqslant \frac{(2m-n)(\Delta-1)^{h-2}}{2}\sqrt{\frac{\Delta}{\delta^h}} \quad (13)$$

Proof. The result is obtained directly from Theorem 1 by noticing that

$$\sum_{i=1}^{n}(\delta_i-1)\sqrt{\delta_i} \geqslant \left(\sum_{i=1}^{n}\delta_i - n\right)\sqrt{\delta} = (2m-n)\sqrt{\delta} \quad (14)$$

and

$$\sum_{i=1}^{n}(\delta_i-1)\sqrt{\delta_i} \leqslant \left(\sum_{i=1}^{n}\delta_i - n\right)\sqrt{\Delta} = (2m-n)\sqrt{\Delta} \quad \square \quad (15)$$

It is well known that for regular graphs of order n, the ordinary Randić index R_1 is equal to $n/2$. From Theorem 1 we immediately arrive at a generalization of this result to the case of the higher-order Randić indices:

Corollary 3. *Let $G = (V, E)$ be a δ-regular graph of girth $g(G)$ and order n. If $\delta \geqslant 2$ and $g(G) > h$, then*

$$R_h(G) = \frac{n}{2}\left(\frac{\delta-1}{\sqrt{\delta}}\right)^{h-1} \quad (16)$$

Theorem 4. *Let $G = (V, E)$ be a bipartite graph of girth $g(G)$ and let $\{V_1, V_2\}$ be the bipartition of V, so that $|V_1| = r$ and $|V_2| = s$. Let $\Delta' = \max_{v\in V_1}\{\delta(v)\}$, $\delta' = \min_{v\in V_1}\{\delta(v)\}$, $\Delta'' = \max_{v\in V_2}\{\delta(v)\}$ and $\delta'' = \min_{v\in V_2}\{\delta(v)\}$. If $\min\{\delta', \delta''\} \geqslant 2$ and $g(G) > h$, then*

$$R_h(G) \leqslant \frac{r(\Delta'-1)^{\lceil h/2\rceil-1}(\Delta''-1)^{\lfloor h/2\rfloor}}{2\sqrt{\delta'^{\lfloor h/2\rfloor-1}\delta''^{\lceil h/2\rceil}}} + \frac{s(\Delta'-1)^{\lfloor h/2\rfloor}(\Delta''-1)^{\lceil h/2\rceil-1}}{2\sqrt{\delta'^{\lceil h/2\rceil}\delta''^{\lfloor h/2\rfloor-1}}} \quad (17)$$

and

$$R_h(G) \geqslant \frac{r(\Delta'-1)^{\lceil h/2\rceil-1}(\delta''-1)^{\lfloor h/2\rfloor}}{2\sqrt{\Delta'^{\lfloor h/2\rfloor-1}\Delta''^{\lceil h/2\rceil}}} + \frac{s(\delta'-1)^{\lfloor h/2\rfloor}(\delta''-1)^{\lceil h/2\rceil-1}}{2\sqrt{\Delta'^{\lceil h/2\rceil}\Delta''^{\lfloor h/2\rfloor-1}}} \quad (18)$$

Proof. If $\min\{\delta', \delta''\} \geqslant 2$, then for every $u \in V$ and $w \in N(u)$ we have $N(w)\setminus\{u\} \neq \emptyset$. So, for every vertex $u \in V$, there exists a sequence $uu_1u_2, \ldots, u_h$ such that $u_1 \in N(u)$, $u_2 \in N(u_1)\setminus\{u\}$, $u_3 \in N(u_2)\setminus\{u_1\}, \ldots$, $u_h \in N(u_{h-1})\setminus\{u_{h-2}\}$. If $g(G) > h$, then the sequence $uu_1u_2, \ldots, u_h$ is a path. Conversely, every path of length h starting at u can be constructed as above.

Suppose that h is even. Then the number of paths of length h starting at a vertex u is bounded by

$$T_h(u) \leqslant \Delta'(\Delta'-1)^{h/2-1}(\Delta''-1)^{h/2}, \quad \forall u \in V_1 \quad (19)$$

and

$$T_h(u) \leqslant \Delta''(\Delta'-1)^{h/2}(\Delta''-1)^{h/2-1}, \quad \forall u \in V_2 \quad (20)$$

Thus, the number of paths of length h in G starting at a vertex belonging to V_1 is bounded by

$$P'_h = \frac{1}{2}\sum_{u\in V_1}T_h(u) \leqslant \frac{1}{2}\left[r\Delta'(\Delta'-1)^{h/2-1}(\Delta''-1)^{h/2}\right] \quad (21)$$

Analogously, the number of paths of length h in G starting at a vertex belonging to V_2 is bounded by

$$P''_h = \frac{1}{2}\sum_{u\in V_2}T_h(u) \leqslant \frac{1}{2}\left[s\Delta''(\Delta'-1)^{h/2}(\Delta''-1)^{h/2-1}\right] \quad (22)$$

Therefore, we have

$$\begin{aligned} R_h &= \sum_{v_{i_1} v_{i_2}, \dots, v_{i_{h+1}} \in \mathscr{P}_h} \frac{1}{\sqrt{\delta(v_{i_1})\delta(v_{i_2}) \cdots \delta(v_{i_{h+1}})}} \\ &\leqslant P'_h \frac{1}{\sqrt{\delta'^{h/2+1} \delta''^{h/2}}} + P''_h \frac{1}{\sqrt{\delta'^{h/2} \delta''^{h/2+1}}} \\ &\leqslant \frac{r\Delta'(\Delta'-1)^{h/2-1}(\Delta''-1)^{h/2}}{2\sqrt{\delta'^{h/2+1}\delta''^{h/2}}} + \frac{s\Delta''(\Delta'-1)^{h/2}(\Delta''-1)^{h/2-1}}{2\sqrt{\delta'^{h/2}\delta''^{h/2+1}}} \\ &= \frac{r(\Delta'-1)^{h/2-1}(\Delta''-1)^{h/2}}{2\sqrt{\delta'^{h/2-1}\delta''^{h/2}}} + \frac{s(\Delta'-1)^{h/2}(\Delta''-1)^{h/2-1}}{2\sqrt{\delta'^{h/2}\delta''^{h/2-1}}} \end{aligned} \quad (23)$$

On the other hand, if h is odd we obtain that the number of paths of length h starting at a vertex u is bounded by

$$T_h(u) \leqslant \Delta'(\Delta'-1)^{(h-1)/2}(\Delta''-1)^{(h-1)/2}, \quad \forall u \in V_1 \quad (24)$$

and

$$T_h(u) \leqslant \Delta''(\Delta'-1)^{(h-1)/2}(\Delta''-1)^{(h-1)/2}, \quad \forall u \in V_2 \quad (25)$$

Now, by proceeding as above we obtain

$$\begin{aligned} R_h &= \sum_{v_{i_1} v_{i_2}, \dots, v_{i_{h+1}} \in \mathscr{P}_h} \frac{1}{\sqrt{\delta(v_{i_1})\delta(v_{i_2}) \cdots \delta(v_{i_{h+1}})}} \\ &\leqslant \frac{r\Delta'(\Delta'-1)^{(h-1)/2}(\Delta''-1)^{(h-1)/2}}{2\sqrt{\delta'^{(h+1)/2}\delta''^{(h+1)/2}}} + \frac{s\Delta''(\Delta'-1)^{(h-1)/2}(\Delta''-1)^{(h-1)/2}}{2\sqrt{\delta'^{(h+1)/2}\delta''^{(h+1)/2}}} \\ &= \frac{r(\Delta'-1)^{(h-1)/2}(\Delta''-1)^{(h-1)/2}}{2\sqrt{\delta'^{(h-3)/2}\delta''^{(h+1)/2}}} + \frac{s(\Delta'-1)^{(h-1)/2}(\Delta''-1)^{(h-1)/2}}{2\sqrt{\delta'^{(h+1)/2}\delta''^{(h-3)/2}}} \end{aligned} \quad (26)$$

By joining (23) and (26) into a single formula we obtain the upper bound stated in Theorem 4. The lower bound is deduced analogously. □

Corollary 5. *Let G be a (δ', δ'')-semiregular bipartite graph with $r+s$ vertices, of girth $g(G)$. If $\min\{\delta', \delta''\} \geqslant 2$ and $g(G) > h$, then*

$$R_h(G) = \frac{r(\delta'-1)^{\lceil h/2\rceil-1}(\delta''-1)^{\lfloor h/2\rfloor}}{2\sqrt{\delta'^{\lfloor h/2\rfloor-1}\delta''^{\lceil h/2\rceil}}} + \frac{s(\delta'-1)^{\lfloor h/2\rfloor}(\delta''-1)^{\lceil h/2\rceil-1}}{2\sqrt{\delta'^{\lceil h/2\rceil}\delta''^{\lfloor h/2\rfloor-1}}} \quad (27)$$

3. Concluding remarks

Both the ordinary Randić index R_1, Eq. (1), and its higher-order congeners R_h, $h > 1$, Eq. (2), are important in chemical applications, when these are computed for molecular graphs. In such applications the vertex degree sequence of the graph is always known, as well as its girth. In this work we obtained lower and upper bounds for R_h in terms of the vertex degree sequence, valid whenever the girth is greater than h. Thus our results make it possible to find a narrow interval for $R_1, R_2, R_3, \dots$, applicable to any chemically relevant type of cyclic or polycyclic molecular graphs.

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