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 $\delta(v)$ be the degree of the vertex $v_i \in V$. If the vertices $v_1, v_2, \ldots, v_h$ form a path of length $h$, $h \geq 1$, in the graph $G$, then the $h$th order Randić index $R_h$ of $G$ is defined as the sum of the terms $1/\sqrt{\delta(v_i)\delta(v_j)\cdots\delta(v_{h+1})}$ 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 $R_8$ are obtained for the case when $G$ is regular or semiregular bipartite.

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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 $\delta_1 \geq \delta_2 \geq \cdots \geq \delta_n$. The maximum and minimum vertex degree will be denoted by $\Delta$ and $\delta$, 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 $\Delta \leq 4$ [1].

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

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

(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 $h \geq 1$, the $h$th order Randić index $R_h(G)$ of a graph $G$ is defined as

$$R_h = R_h(G) = \sum_{v_i, v_j, \ldots, v_{h+1} \in V} \frac{1}{\sqrt{\delta(v_i)\delta(v_j)\cdots\delta(v_{h+1})}}$$

(2)

where $\mathcal{P}_h$ 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,

$$R_0 \leq \frac{n_h + c_h}{2} \left(\frac{\Delta - 1}{\Delta}\right)^{h-1}$$

(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 $\Phi$ whose $(i,j)$-entry is

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

(4)

where $v_i \sim v_j$ 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 $\Phi$, then there is a following relation between $R_2$ and $R_1$ [13]:

$$R_2 \geq \frac{4(2R_1 - \phi)^2}{n - \phi} + \phi - \tau \sqrt{\delta}$$

(5)

where

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

(6)
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 fullerences are regular of degree 3. A bipartite graph is said to be semiregular (of degrees $r^-$, $r^+$) if any two adjacent vertices $u, v$ it holds $\delta(u) = r^-$ and $\delta(v) = r^+$. 

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 $\delta_1 \geq \delta_2 \geq \cdots \geq \delta_n, \; \delta_1 = \delta, \; \delta_n = \delta$. If $\delta \geq 2$ and $g(G) > h$, then

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

**Proof.** Since $\delta \geq 2$, for every $v \in V$, the number of paths of length 2 in $G$ of the form $v_1v_2v_3$ is $\delta(v)(\delta(v) - 1)/2$. So, we have

$$R_2 = \sum_{v_1v_2v_3 \in E} 1 = \frac{1}{\delta(v)} \sum_{i=1}^{n} \frac{\delta(v_i)(\delta(v_i) - 1)}{2} \leq \frac{1}{\sqrt{\delta}} \sum_{i=1}^{n} \delta(v_i) \; (8)$$

and

$$R_2 = \sum_{v_1v_2v_3 \in E} 1 \leq \frac{1}{\delta(v)} \sum_{i=1}^{n} \frac{\delta(v_i)(\delta(v_i) - 1)}{2} \leq \frac{1}{\sqrt{\delta}} \sum_{i=1}^{n} \delta(v_i) \; (9)$$

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

Suppose now that $h \geq 3$. Given a vertex $u \in V$, let $\mathcal{P}_h(u)$ be the set of paths of length $h$ whose second vertex is $u$, that is, paths of the form $u_1u_2u_3 \ldots u_h$. 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 $\delta \geq 2$, 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 $u_1u_2u_3 \ldots u_h$ such that $u_1, \; u_2 \in N(u), \; \ldots, \; u_h \in N(u_{h-1}) \setminus \{u_{h-2}\}$. If $g(G) > h$, then the sequence $u_1u_2u_3 \ldots u_h$ 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

$$|\mathcal{P}_h(u)| \geq \min_{u_1u_2u_3 \ldots u_h \in \mathcal{P}_h(u)} \left\{ \delta(u)(\delta(u) - 1) \prod_{j=2}^{h-1} (\delta(u_j) - 1) \right\} \geq \delta(u)(\delta(u) - 1)(\delta - 1)^{h-3} \; (10)$$

and

$$|\mathcal{P}_h(u)| \leq \max_{u_1u_2u_3 \ldots u_h \in \mathcal{P}_h(u)} \left\{ \delta(u)(\delta(u) - 1) \prod_{j=2}^{h-1} (\delta(u_j) - 1) \right\} \leq \delta(u)(\delta(u) - 1)(\delta - 1)^{h-3} \; (11)$$

The higher-order Randić index of $G$ is bounded by

$$\frac{1}{2} \sum_{u \in V} |\mathcal{P}_h(u)| \leq R_h(G) \leq \frac{1}{2} \sum_{u \in V} |\mathcal{P}_h(u)| \frac{1}{\sqrt{\delta(u)} \sqrt{\delta(u)}} \; (12)$$

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 $\delta$ and maximum degree $\Delta$. If $\delta \geq 2$ and $g(G) > h$, then

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

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

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

and

$$\sum_{i=1}^{n} (\delta_i - 1) \delta_i \leq \left( \sum_{i=1}^{n} (\delta_i - n) \right) \Delta = (2m - n)\Delta \; \Box \; (15)$$

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 $\delta$-regular graph of girth $g(G)$ and order $n$. If $\delta \geq 2$ and $g(G) > h$, then

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

**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 $A' = \max_{u \in V_1}\{\delta(u)\}$, $A'' = \min_{u \in V_1}\{\delta(u)\}$, $A' = \max_{u \in V_2}\{\delta(u)\}$ and $A'' = \min_{u \in V_2}\{\delta(u)\}$. If $\min\{\delta', \delta''\} \geq 2$ and $g(G) > h$, then

$$R_h(G) \leq \frac{r(A' - 1)^{h-2}(A'' - 1)^{h-2}}{2\sqrt{\delta}^{(h-2)}(A' + 1)^{h-2}} + \frac{s(A' - 1)^{h-2}(A'' - 1)^{h-2}}{2\sqrt{\delta}^{(h-2)}(A'' + 1)^{h-2}} \; (17)$$

and

$$R_h(G) \geq \frac{r(A' - 1)^{h-2}(A'' - 1)^{h-2}}{2\sqrt{\delta}^{(h-2)}(A' + 1)^{h-2}} + \frac{s(A' - 1)^{h-2}(A'' - 1)^{h-2}}{2\sqrt{\delta}^{(h-2)}(A'' + 1)^{h-2}} \; (18)$$

**Proof.** If $\min\{\delta', \delta''\} \geq 2$, then for every $u \in V$ and $w \in N(u)$ we have $N(w) \setminus \{v\} \neq \emptyset$. So, for every vertex $u \in V$, there exists a sequence $u_1u_2u_3 \ldots u_h$ such that $u_1, \; u_2 \in N(u), \; \ldots, \; u_h \in N(u_{h-1}) \setminus \{u_{h-2}\}$. If $g(G) > h$, then the sequence $u_1u_2u_3 \ldots u_h$ 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

$$T_h(u) \leq A'(A' - 1)^{h-2}(A'' - 1)^{h/2}, \; \forall u \in V_1 \; (19)$$

and

$$T_h(u) \leq A''(A'' - 1)^{h-2}(A'' - 1)^{h/2}, \; \forall u \in V_2 \; (20)$$

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

$$P'_h = \frac{1}{2} \sum_{u \in V_1} \frac{1}{\sqrt{\delta(u)} \sqrt{\delta(u)}} \leq R_h(G) \leq \frac{1}{2} \sum_{u \in V_1} \frac{1}{\sqrt{\delta(u)} \sqrt{\delta(u)}} \; (21)$$

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

$$P''_h = \frac{1}{2} \sum_{u \in V_2} \frac{1}{\sqrt{\delta(u)} \sqrt{\delta(u)}} \leq R_h(G) \leq \frac{1}{2} \sum_{u \in V_2} \frac{1}{\sqrt{\delta(u)} \sqrt{\delta(u)}} \; (22)$$
Therefore, we have
\[ R_h = \sum_{v_1, v_2, \ldots, v_{h+1} \in V} \frac{1}{\sqrt{\delta(v_1) \delta(v_2) \cdots \delta(v_{h+1})}} \]
\[ \leq P_h \sqrt{\delta^{h+2}/2 \delta^{h+1}/2} + P_h \sqrt{\delta^{h+2}/2 \delta^{h+1}/2} \]
\[ \leq \frac{r(A' - 1)^{h+1/2}(A' - 1)^{h-1/2}}{2 \sqrt{\delta^{h+1}/2 \delta^{h+1}/2}} + \frac{s(A' - 1)^{h+1/2}(A' - 1)^{h-1/2}}{2 \sqrt{\delta^{h+1}/2 \delta^{h+1}/2}} \]
\[ = \frac{r(A' - 1)^{h+1/2}(A' - 1)^{h-1/2}}{2 \sqrt{\delta^{h+1}/2 \delta^{h+1}/2}} + \frac{s(A' - 1)^{h+1/2}(A' - 1)^{h-1/2}}{2 \sqrt{\delta^{h+1}/2 \delta^{h+1}/2}} \]
\[ = \frac{r(A' - 1)^{h+1/2}(A' - 1)^{h-1/2}}{2 \sqrt{\delta^{h+1}/2 \delta^{h+1}/2}} + \frac{s(A' - 1)^{h+1/2}(A' - 1)^{h-1/2}}{2 \sqrt{\delta^{h+1}/2 \delta^{h+1}/2}} \text{(23)} \]
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
\[ T_h(u) \leq \frac{A'(A' - 1)^{h-1/2}(A' - 1)^{h+1/2}}{2} \quad \forall u \in V_1 \]  
(24)
and
\[ T_h(u) \leq \frac{A'(A' - 1)^{h-1/2}(A' - 1)^{h+1/2}}{2} \quad \forall u \in V_2 \]  
(25)
Now, by proceeding as above we obtain
\[ R_h = \sum_{v_1, v_2, \ldots, v_{h+1} \in V} \frac{1}{\sqrt{\delta(v_1) \delta(v_2) \cdots \delta(v_{h+1})}} \]
\[ \leq \frac{r(A' - 1)^{h+1/2}(A' - 1)^{h-1/2}}{2 \sqrt{\delta^{h+1}/2 \delta^{h+1}/2}} + \frac{s(A' - 1)^{h+1/2}(A' - 1)^{h-1/2}}{2 \sqrt{\delta^{h+1}/2 \delta^{h+1}/2}} \]
\[ = \frac{r(A' - 1)^{h+1/2}(A' - 1)^{h-1/2}}{2 \sqrt{\delta^{h+1}/2 \delta^{h+1}/2}} + \frac{s(A' - 1)^{h+1/2}(A' - 1)^{h-1/2}}{2 \sqrt{\delta^{h+1}/2 \delta^{h+1}/2}} \text{(26)} \]
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 \( (\delta', \delta'') \)-semiregular bipartite graph with \( r + s \) vertices, of girth \( g(G) \). If \( m(\delta', \delta'') \geq 2 \), and \( g(G) > h \), then
\[ R_h(G) = \frac{r(\delta' - 1)^{h+1/2}(\delta' - 1)^{h+1/2}}{2 \sqrt{\delta^{h+1}/2 \delta^{h+1}/2}} + \frac{s(\delta' - 1)^{h+1/2}(\delta' - 1)^{h+1/2}}{2 \sqrt{\delta^{h+1}/2 \delta^{h+1}/2}} \]  
(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 \( R_1, R_2, R_3, \ldots \), applicable to any chemically relevant type of cyclic or polycyclic molecular graphs.

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**References**