ON MOLECULAR GRAPHS WITH SMALLEST AND GREATEST ZEROOTH-ORDER GENERAL RANDIĆ INDEX

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Abstract

A molecular \((n,m)\)-graph \(G\) is a connected simple graph with \(n\) vertices, \(m\) edges and vertex degrees not exceeding 4. If \(d(v)\) denotes the degree of the vertex \(v\), then the zeroth-order general Randić index \(0R_\alpha\) of the graph \(G\) is defined as \(\sum_{v \in V(G)} d(v)^\alpha\), where \(\alpha\) is a pertinently chosen real number. We characterize, for any \(\alpha\), the molecular \((n,m)\)-graphs with smallest and greatest \(0R_\alpha\).

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1 Introduction

The Randić (or connectivity) index was introduced by Randić in 1975 and is defined as [25]

\[ R = R(G) = \sum_{uv \in E(G)} (d(u) d(v))^{-\frac{1}{2}} \]

where \( d(u) \) denotes the degree of the vertex \( u \) of the graph \( G \), and \( E(G) \) is the edge set of \( G \). Randić himself demonstrated [25] that this index is well correlated with a variety of physico-chemical properties of various classes of organic compounds. Eventually, this structure-descriptor became one of the most popular topological indices to which two books [15, 17], several reviews [7, 24, 26] and countless research papers are devoted.

Like other successful structure-descriptors, the Randić index received considerable attention also from mathematical chemists and mathematicians. In particular, bounds for \( R \) and graphs extremal with regard to \( R \) were extensively studied [1, 2, 4, 8, 9, 10, 11, 12].

In 1998 Bollobás and Erdős [3] generalized \( R(G) \) by replacing the exponent \(-\frac{1}{2}\) by an arbitrary real number \( \alpha \). This graph invariant is called the general Randić index and will be denoted by \( R_\alpha = R_\alpha(G) \). Li and Yang [20] studied \( R_\alpha \) for general \( n \)-vertex graphs, obtained lower and upper bounds for it, and characterized the corresponding extremal graphs. Later Hu, Li and Yuan [13, 14] determined the trees extremal with regard to \( R_\alpha \), whereas Li, Wang and Wei [19] gave lower and upper bounds for \( R_\alpha \) of molecular \((n, m)\)-graphs. Other mathematical studies of the general Randić index are found in [5, 6].

The zeroth-order Randić index, conceived by Kier and Hall [16], is

\[ 0^o R = 0^o R(G) = \sum_{v \in V(G)} d(v)^{-\frac{1}{2}} \]

Eventually, Li and Zheng [22] defined the zeroth-order general Randić index of a graph \( G \) as

\[ 0^o R_\alpha = 0^o R_\alpha(G) = \sum_{v \in V(G)} d(v)^\alpha \]
for any real number \( \alpha \). 

Pavlović determined the graphs with maximum \( 0R \)-index [23]. Li et al. [18] investigated the same problem for the topological index \( M_1(G) \), one of the Zagreb indices, that is defined as \( M_1(G) = \sum_{v \in V(G)} d(v)^2 \). (Evidently, \( M_1 \equiv 0R_\alpha \) for \( \alpha = +2 \).) They obtained sufficient and necessary conditions under which \((n, m)\)-graphs have minimum \( M_1 \), and a necessary condition for an \((n, m)\)-graph having maximum \( M_1(G) \). Li and Zhao [21] characterized trees with the first three smallest and largest zeroth-order general Randić index, with the exponent \( \alpha \) being equal to \( k, -k, 1/k, \) and \(-1/k\), where \( k \geq 2 \) is an integer.

In this paper we investigate the zeroth-order general Randić index of molecular \((n, m)\)-graphs, i.e., connected simple graphs with \( n \) vertices, \( m \) edges and maximum vertex degree at most 4. We characterize the molecular \((n, m)\)-graphs with extremal (maximum or minimum) zeroth-order general Randić index.

First we need to introduce some notation.

Denote by \( D(G) = [d_1, d_2, \cdots, d_n] \) the degree sequence of the graph \( G \), where \( d_i \) stands the degree of the \( i \)-th vertex of \( G \), and \( d_1 \geq d_2 \geq \cdots \geq d_n \).

If there is a graph \( G \), such that \( d_i \geq d_j + 2 \), let \( G' \) be the graph obtained from \( G \) by replacing the pair \( (d_i, d_j) \) by the pair \( (d_i - 1, d_j + 1) \). In other words, if \( D(G) = [d_1, d_2, \cdots, d_{i-1}, d_i, d_{i+1}, \cdots, d_{j-1}, d_j, d_{j+1}, \cdots, d_n] \), then \( D(G') = [d_1, d_2, \cdots, d_{i-1}, d_i - 1, d_{i+1}, \cdots, d_{j-1}, d_j + 1, d_{j+1}, \cdots, d_n] \).

Note that if \( \alpha = 0 \) then \( 0R_\alpha(G) = n \), and if \( \alpha = 1 \) then \( 0R_\alpha(G) = 2m \). Therefore, in the following we always assume that \( \alpha \neq 0, 1 \).

**Lemma 1.1** For the two graphs \( G \) and \( G' \), specified above, we have

(i) \( 0R_\alpha(G) > 0R_\alpha(G') \) for \( \alpha < 0 \) or \( \alpha > 1 \)

(ii) \( 0R_\alpha(G) < 0R_\alpha(G') \) for \( 0 < \alpha < 1 \).
Proof. Since $0R_\alpha(G) = \sum_{v \in V(G)} d(v)^\alpha$, we have

$$0R_\alpha(G) - 0R_\alpha(G') = d_i^\alpha + d_j^\alpha - (d_i - 1)^\alpha - (d_j + 1)^\alpha$$

$$= [d_i^\alpha - (d_i - 1)^\alpha] - [(d_j + 1)^\alpha - d_j^\alpha]$$

$$= \alpha (\xi_1^{\alpha-1} - \xi_2^{\alpha-1})$$

where $\xi_1 \in (d_i - 1, d_i)$, and $\xi_2 \in (d_j, d_j + 1)$. So, by $d_i \geq d_j + 2$, we have $\xi_1 > \xi_2$. Then $0R_\alpha(G) > 0R_\alpha(G')$ for $\alpha < 0$ or $\alpha > 1$, whereas $0R_\alpha(G) < 0R_\alpha(G')$ for $0 < \alpha < 1$.

\[\Box\]

2 Extremal molecular $(n, m)$-graphs

Denote by $n_i$ the number of vertices of degree $i$ in a molecular $(n, m)$-graph $G$. Then we have

$$0R_\alpha(G) = n_1 + 2^\alpha n_2 + 3^\alpha n_3 + 4^\alpha n_4 \quad (2.1)$$

Theorem 2.1 Let $C^*$ be a molecular $(n, m)$-graph with degree sequence $[d_1, d_2, \cdots, d_n]$, such that $|d_i - d_j| \leq 1$ for any $i \neq j$. Then for $\alpha < 0$ or $\alpha > 1$, $C^*$ has the minimum zeroth-order general Randić index among all molecular $(n, m)$-graphs, whereas for $0 < \alpha < 1$, $C^*$ has the maximum zeroth-order general Randić index among all molecular $(n, m)$-graphs. Moreover,

$$0R_\alpha(C^*) = \begin{cases} 
2 + 2^\alpha (n - 2) & \text{if } m = n - 1 \\
2^\alpha (3n - 2m) + 3^\alpha (2m - 2n) & \text{if } n \leq m \leq \lfloor 3n/2 \rfloor \\
3^\alpha (4n - 2m) + 4^\alpha (2m - 3n) & \text{if } \lfloor 3n/2 \rfloor < m \leq 2n
\end{cases}$$

Proof. We only consider the case $0 < \alpha < 1$, because the proof for the other case is fully analogous. Let $G$ be a molecular graph and $D(G) = [d_1, d_2, \cdots, d_n]$. If $G \not\cong C^*$, then there must exist a pair $(d_i, d_j)$ such that $d_i \geq d_j + 2$. By Lemma 1.1, the graph $G'$, obtained by replacing the pair $(d_i, d_j)$ by the pair $(d_i - 1, d_j + 1)$, has a greater $0R_\alpha$-value than $G$. Consequently, $G$ is not a molecular $(n, m)$-graph with maximum zeroth-order general Randić index.
To show the existence, we construct the extremal \((n, m)\)-graph \(C^*\) (with minimum \(^0R_{\alpha}\) for \(\alpha < 0\) or \(\alpha > 1\), and with maximum \(^0R_{\alpha}\) for \(0 < \alpha < 1\)) by adding edges one by one. First, we start from a tree. There must be at least two 1-degree vertices in a tree. By Lemma 1.1, there does not exist any 3-degree vertex, and so the extremal tree must be the path \(P_n\). Next we add an edge joining the two leaves of the path. In this way the degrees of all vertices become equal to two, and then we get a cycle. We continue by adding edges one by one, so as to maximize the number of 3-degree vertices, until either there remain no 2-degree vertices, or remains exactly one. If more edges need to be added, then we first connect the 2-degree vertex (if such does exist) with a non-adjacent 3-degree vertex, and continue by connecting pairs of nonadjacent 3-degree vertices. The construction is shown in Figure 2.1.

![Figure 2.1 Constructing molecular graphs with extremal zeroth-order general Randić index, according to Theorem 2.1.](image)

**Theorem 2.2** Let \(G^*\) be a molecular \((n, m)\)-graph with at most one vertex of degree 2 or 3. If one of the following conditions holds:

(I) \(m = n - 1\)

(II) \(m \geq n \geq 6\), for \(n = 6\), \(m \geq 10\), and for \(n = 7\), \(m \neq 8\)

then for \(\alpha < 0\) or \(\alpha > 1\), \(G^*\) has the maximum zeroth-order general Randić index among all molecular \((n, m)\)-graphs, whereas for \(0 < \alpha < 1\), the same graph has the minimum zeroth-order general Randić index among all molecular \((n, m)\)-graphs. Moreover,

\[
^0R_{\alpha}(G^*) = \begin{cases} 
(4n - 2m)/3 + 4^\alpha (2m - n)/3 & \text{if } 2m - n \equiv 0 \pmod{3} \\
(4n - 2m - 2)/3 + 2^\alpha + 4^\alpha (2m - n - 1)/3 & \text{if } 2m - n \equiv 1 \pmod{3} \\
(4n - 2m - 1)/3 + 3^\alpha + 4^\alpha (2m - n - 2)/3 & \text{if } 2m - n \equiv 2 \pmod{3}
\end{cases}
\]
Proof. Again, we only consider the case $0 < \alpha < 1$, because the proof for the other case is similar. Let $G'$ be a molecular $(n, m)$-graph and $D(G') = [d_1, d_2, \cdots, d_n]$. Let $G'$ possess two vertices of degree 2 or 3, i.e., let there be a pair $(d_i, d_j)$, such that $3 \geq d_i \geq d_j \geq 2$. Then by Lemma 1.1, there is a graph $G$, obtained by replacing the pair $(d_i, d_j)$ by the pair $(d_i+1, d_j-1)$, that has a smaller $0R_\alpha$-value than $G'$. Repeating the above operation until there is no pair $(d_i, d_j)$, such that $3 \geq d_i \geq d_j \geq 2$, we arrive at $G^*$ with minimum zeroth-order general Randić index. In view of (2.1), for $G^*$ we have

$$\begin{cases}
  n_1 + n_2 + n_3 + n_4 &= n \\
  n_1 + 2n_2 + 3n_3 + 4n_4 &= 2m \\
  n_2 + n_3 &\leq 1
\end{cases}$$

From the above equations, we have one of the following three options:

(1) $n_2 = n_3 = 0$, implying $n_1 = (4n - 2m)/3$, $n_4 = (2m - n)/3$, and $2m - n \equiv 0 \pmod{3}$

(2) $n_2 = 1$, $n_3 = 0$, implying $n_1 = (4n - 2m - 2)/3$, $n_4 = (2m - n - 1)/3$, and $2m - n \equiv 1 \pmod{3}$

(3) $n_2 = 0$, $n_3 = 1$, implying $n_1 = (4n - 2m - 1)/3$, $n_4 = (2m - n - 2)/3$, and $2m - n \equiv 2 \pmod{3}$.

In order to show the existence, we construct $G^*$ by distinguishing the following cases:

(I) $m = n - 1$, i.e., $G^*$ is a tree.

(I.1) If $2m - n \equiv 0 \pmod{3}$, we first construct a path with $n_4$ vertices, and then add $n_1$ pendent vertices, taking care that no vertex gets degree greater than 4.

(I.2) If $2m - n \equiv 1 \pmod{3}$, we first construct a path with $n_4$ vertices, then add $n_1$ pendent vertices, taking care that no vertex gets degree greater than 4, and finally subdivide an edge by inserting to it a vertex of degree 2.

(I.3) If $2m - n \equiv 2 \pmod{3}$, we first construct a path with $n_4 + 1$ vertices, and then add $n_1$ pendent vertices, taking care that no vertex gets degree greater than 4.
(II) $m \geq n \geq 6$, for $n = 6$ and $m \geq 10$, or for $n = 7$ and $m \neq 8$.

In Figure 2.2 we show one of the possible graphs $G^*$ for $n_4 \leq 4$, that is for $[(2m - n)/3] \leq 4$. For $n_4 \geq 5$, we construct $G^*$ as follows:

(II.1) If $2m - n \equiv 0 \pmod{3}$, we first construct a 4-regular graph on $n_4$ vertices, then delete $n_1/2$ edges from it, and then add $n_1$ pendent vertices, taking care that no vertex gets degree greater than 4.

(II.2) If $2m - n \equiv 1 \pmod{3}$, we first construct a 4-regular graph on $n_4$ vertices, then delete $n_1/2$ edges from it, then add $n_1$ pendent vertices, taking care that no vertex gets degree greater than 4, and finally subdivide an edge inserting to it a vertex of degree 2.

(II.3) If $2m - n \equiv 2 \pmod{3}$, we first construct a 4-regular graph on $n_4 + 1$ vertices, then delete $(n_1 + 1)/2$ edges from it, and then add $n_1$ pendent vertices, taking care that no vertex gets degree greater than 4.

This completes the proof.

Note that Theorem 2.2 holds under the conditions $m = n - 1$, or $n = 6$ and $m \geq 10$, or $n = 7$ and $m \neq 8$, or $m \geq n \geq 8$, since for the other pairs of $n$ and $m$ the extremal degree sequences obtained in Theorem 2.2 are not graphic. It is easy to check that for $n = 1, 2, 3$, and for $n \geq 4$ and $m = \binom{n}{2} - 1$ or $m = \binom{n}{2}$ the $(n,m)$-graph is unique. For $n = 4$ and $m = 4$, or $n = 5$ and $5 \leq m \leq 8$, or $n = 6$ and $6 \leq m \leq 9$, or $n = 7$ and $m = 8$ we can characterize the extremal graphs by examining all possible degree sequences. These extremal graphs are depicted in Figure 2.3 (minimum ones for $0 < \alpha < 1$, maximum ones for $\alpha < 0$ or $\alpha > 1$, except for $n = 5$ and $m = 7$, in which case (a) is the minimum graph for $0 < \alpha < 1$ and maximum graph for $\alpha < 0$ or $1 < \alpha < 2$, and (b) is the maximum graph for $\alpha \geq 2$).
Figure 2.2 Molecular graphs with extremal zeroth-order general Randić index, having four or fewer vertices of degree 4.
Figure 2.3 Some graphs with extremal zeroth-order general Randić index; for details see text.

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