Available online at www.sciencedirect.com
ScienceDirect
Discrete Applied Mathematics 155 (2007) 1044 – 1054
DISCRETE APPLIED MATHEMATICS
www.elsevier.com/locate/dam

Connected (n, m)-graphs with minimum and maximum zeroth-order general Randić index☆

Yumei Hu[a,b], Xueliang Li[a], Yongtang Shi[a], Tianyi Xu[a]

[a] *Center for Combinatorics and LPMC, Nankai University, Tianjin 300071, PR China*
[b] *Department of Mathematics, Tianjin University, Tianjin 300072, PR China*

Received 5 April 2006; received in revised form 14 November 2006; accepted 26 November 2006
Available online 17 January 2007

Abstract

Let G be a graph and $d(v)$ denote the degree of a vertex v in G. Then the zeroth-order general Randić index ${}^0R_\alpha(G)$ of the graph G is defined as $\sum_{v\in V(G)} d(v)^\alpha$, where α is a pertinently chosen real number. We characterize, for any α, the connected (n, m)-graphs with minimum and maximum ${}^0R_\alpha$.

Keywords: Molecular structure descriptor; Zetoth-order general Randić index; Extremal (n, m)-graph; Degree sequence

1. Introduction

For a (molecular) graph $G = (V, E)$, the *general Randić index* $R_\alpha(G)$ of G is defined as the sum of $(d_G(u)d_G(v))^\alpha$ over all edges uv of G where $d_G(u)$ denotes the degree of $u \in V$, i.e.,

$$R_\alpha(G) = \sum_{uv\in E(G)} (d_G(u)d_G(v))^\alpha,$$

where α is an arbitrary real number.

It is well known that $R_{-1/2}$ was introduced by Randić [17] in 1975 as one of the many graph-theoretical parameters derived from the graph underlying some molecule. Like other successful chemical indices, this index has been closely correlated with many chemical properties. The general Randić index was proposed by Bollobás and Erdös [2], and Amic et al. [1], independently, in 1998. Then it has been extensively studied by both mathematicians and theoretical chemists [9]. Many important mathematical properties have been established [5]. For a survey of results, we refer to the new book written by Li and Gutman [12].

In 2004, Li and Yang [13] studied the general Randić index for general graphs, and they obtained lower and upper bounds for the general Randić index among graphs of order n, and the corresponding extremal graphs. Later Hu et al. [7,8] showed the trees with extremal general Randić index.

The zeroth-order Randić index defined by Kier and Hall [10] is ${}^0R = \sum_{u\in V(G)} d(u)^{-1/2}$. Pavlović [16] gave a graph with the maximum value of ${}^0R(G)$. In [11], Li et al. investigated the same problem for the topological index $M_1(G)$, a

☆ Supported by NSFC and the “973” project.
E-mail address: lxl@nankai.edu.cn (X. Li).

0166-218X/$ - see front matter © 2006 Elsevier B.V. All rights reserved.
doi:10.1016/j.dam.2006.11.008

Zagreb index, which is defined as $M_1(G)=\sum_{v\in V(G)} d(u)^2$. They gave a sufficient and necessary condition for (n,m)-graphs with minimum Zagreb index, and a necessary condition for (n,m)-graphs with maximum Zagreb index. Later Li and Zheng [15] defined the zeroth-order general Randić index ${}^0R_\alpha(G)$ of a graph G as ${}^0R_\alpha(G)=\sum_{v\in V(G)} d(u)^\alpha$ for general real number α. In [14] Li and Zhao characterized trees with the first three minimum and maximum values of zeroth-order general Randić index, with the exponent equal to m, $-m$, $1/m$ and $-1/m$, where $m\geqslant 2$ is an integer.

In our another paper [6] we investigated the zeroth-order general Randić index for molecular (n,m)-graphs, i.e., simple connected graphs with n vertices, m edges and maximum degree at most 4. In this paper, we investigate the zeroth-order general Randić index for general simple connected (n,m)-graphs. We characterize the simple connected (n,m)-graphs with extremal (maximum and minimum) zeroth-order general Randić index.

2. Definitions and notations

The set of vertices and edges of a simple graph G are denoted by $V(G)$ and $E(G)$, respectively. The order of G is defined by $|V(G)|$ and the size of G is defined by $|E(G)|$. Denote by $d(u)$ and $N(u)$ the degree and neighborhood of a vertex u, respectively. The *minimum degree* of G is denoted by $\delta(G)$ and the *maximum degree* of G is denoted by $\Delta(G)$. Denote by $D(G)=[d_1,d_2,\ldots,d_n]$ the degree sequence of the graph G, where d_i stands for the degree of the ith vertex of G, and $d_1\geqslant d_2\geqslant\cdots\geqslant d_n$. A vertex of degree i is also called an *i-degree vertex*.

A graph G is *nearly regular* if $|\Delta(G)-\delta(G)|\leqslant 1$, and in this case the degree sequence $D(G)$ is called a *nearly regular* degree sequence. Note that, for given order n and size m, the nearly regular graph, which, denoted by $C^*(n,m)$, is a class of connected graphs, but they have the same ${}^0R_\alpha$-value.

To show the existence, we can get a nearly regular graph with given order n and size m by adding edges one by one. First, we start from a tree ($m=n-1$). There must be at least two 1-degree vertices in a tree. There does not exist any 3-degree vertex, and so the nearly regular graph must be a path P_n. Next we add an edge joining the two leaves of the path. In this way the degrees of the vertices are all equal to two, and then we get a cycle. Then we add edges one by one, so as to maximize the number of 3-degree vertices, until there are no 2-degree vertices. We continue to add edges in this way until we arrive at a complete graph (Fig. 1).

Let $G(n,m)$ be a simple connected graph with n vertices and m edges. A graph $G(n,m)$ is specially denoted by L^* (as described in [16]) if it can be constructed as follows: for $m=n-1$, it is a star. We then add a new edge for $m=n$ between two vertices of degree 1 in the star and get a clique on three vertices. Add one more edge for $m=n+1$ between a vertex out of the clique and some vertices in the clique to increase the degree of this vertex by 1 until it is joined to all the vertices of the clique. We get a clique on four vertices. For $m=n+2,n+3,\ldots$ we continue to add edges in this way until we arrive at a complete graph (Fig. 2). Then we have $m=n+k(k-3)/2+p$, where k $(2\leqslant k\leqslant n-1)$ denotes the number of vertices in the clique, and p denotes the number of vertices with degree k. It is easy to see that k and p satisfy

$$\frac{k^2-3k}{2}\leqslant m-n<\frac{(k+1)^2-3(k+1)}{2}$$

and $0\leqslant p\leqslant k-2$.

For convenience, we introduce a family of graphs which is denoted by $\mathscr{F}$. As described in [3], let $N<n$ be a positive integer, and $d_1,d_2,\ldots,d_N$ be a sequence of positive integers. The graph $G(d_1,d_2,\ldots,d_N)$ has vertex set defined as the disjoint union

$$\bigcup_{0\leqslant j\leqslant N} I_j,$$

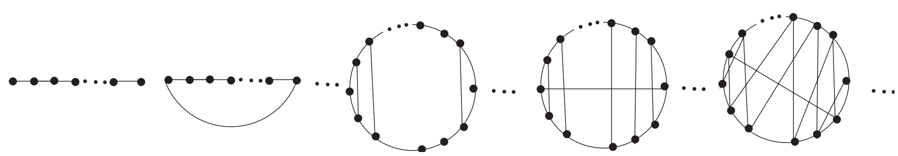

Fig. 1.

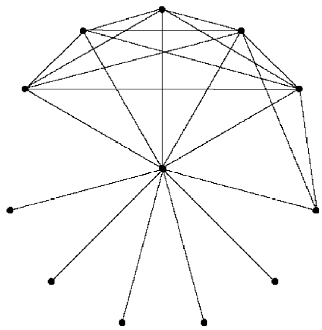

Fig. 2. $L^*(12, 23)$, $k = 6$, $p = 2$.

where $I_0 = \{v_1, v_2, \ldots, v_N\}$, $|I_j| = d_j - d_{j+1}$ for $1 \leqslant j \leqslant N-1$ and $|I_N| = d_N - (N-1)$. For $1 \leqslant j \leqslant N$ we arrange that

$$N(v_j) = (I_0 - \{v_j\}) \cup \left(\bigcup_{j \leqslant k \leqslant N} I_k \right) \quad \text{and} \quad E\left(G\left[\bigcup_{1 \leqslant j \leqslant N} I_j \right] \right) = \emptyset,$$

so that $d(v_j) = d_j$ for all j and $e(G(d_1, d_2, \ldots, d_N)) = \sum_{i=1}^{N} d_i - \binom{N}{2}$. We will, of course, always have $d_1 \geqslant d_2 \geqslant \cdots \geqslant d_N \geqslant N-1$. Each of these graphs of order n, say, is the unique realization of a sequence corresponding to a vertex of the polytope K^n of degree sequences in E^n. Let $\mathscr{F}$ denote the family of graphs of the form $G(d_1, d_2, \ldots, d_N)$ for $d_1 \geqslant d_2 \geqslant \cdots \geqslant d_N \geqslant N-1$. From the definition of $\mathscr{F}$, we have $L^* \in \mathscr{F}$.

Undefined notations and terminologies can be found in [4].

3. Extremal (n, m)-graphs

Note that if $\alpha = 0$ then ${}^0R_\alpha(G) = n$, and if $\alpha = 1$ then ${}^0R_\alpha(G) = 2m$. Therefore, in what follows we always assume that $G(n, m)$ is a simple connected graph and $\alpha \neq 0, 1$.

For convenience, we call G a *minimum* (*maximum*) (n, m)*-graph*, if G has the minimum (maximum) zeroth-order general Randić index among all connected (n, m)-graphs.

If there is a graph G such that $d_i \geqslant d_j + 2$, let $\tilde{G}$ 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 $D(G) = [d_1, d_2, \ldots, d_{i-1}, d_i, d_{i+1}, \ldots, d_{j-1}, d_j, d_{j+1}, \ldots, d_n]$, then $D(\tilde{G}) = [d_1, d_2, \ldots, d_{i-1}, d_i - 1, d_{i+1}, \ldots, d_{j-1}, d_j + 1, d_{j+1}, \ldots, d_n]$.

Lemma 3.1. (Hu et al. [6]) *For the graphs G and $\tilde{G}$, we have*

(i) ${}^0R_\alpha(G) > {}^0R_\alpha(\tilde{G})$, *for* $\alpha < 0$ *or* $\alpha > 1$;
(ii) ${}^0R_\alpha(G) < {}^0R_\alpha(\tilde{G})$, *for* $0 < \alpha < 1$.

Theorem 3.2. *For $\alpha < 0$ or $\alpha > 1$, a minimum (n, m)-graph G is a nearly regular graph C^*; whereas for $0 < \alpha < 1$, a maximum (n, m)-graph G is a nearly regular graph C^*. The extremal value is ${}^0R_\alpha(C^*) = (2m - ns)(s+1)^\alpha + [n(s+1) - 2m]s^\alpha$, where s denotes the minimum degree of C^*.*

Proof. We take the case $0 < \alpha < 1$ for instance, because the proof for the other case is fully analogous. In this case we want to determine the maximum (n, m)-graph.

A degree sequence $D' = [d'_1, d'_2, \ldots, d'_n]$ is *better* than $D = [d_1, d_2, \ldots, d_n]$, if $\sum_{i=1}^{n} d_i^\alpha < \sum_{i=1}^{n} d_i'^\alpha$. It is obviously that if there is a degree sequence $D(G) = [d_1, d_2, \ldots, d_{i-1}, d_i, d_{i+1}, \ldots, d_{j-1}, d_j, d_{j+1}, \ldots, d_n]$, such that $d_i \geqslant d_j + 2$ for some i and j, then the degree sequence $D' = [d_1, d_2, \ldots, d_{i-1}, d_i - 1, d_{i+1}, \ldots, d_{j-1}, d_j + 1, d_{j+1}, \ldots, d_n]$ is better than D.

Let G be a maximum (n, m)-graph and $D(G) = [d_1, d_2, \ldots, d_n]$. If G is not a nearly regular graph, then there must exist a pair (d_i, d_j) such that $d_i \geqslant d_j + 2$. By replacing the pair (d_i, d_j) by the pair $(d_i - 1, d_j + 1)$, we can get another degree sequence D' better than $D(G)$. We continue to replace pairs of degree sequences in this way until we arrive at a nearly regular degree sequence $\tilde{D}$. Note that the nearly regular degree sequence must be graphic, i.e., there is a connected (n, m)-graph $\tilde{G}$ with this nearly regular degree sequence as its degree sequence. Clearly, ${}^0R_\alpha(G) < {}^0R_\alpha(\tilde{G})$, which leads to a contradiction. □

Now we will show that maximum (n, m)-graphs must belong to the family $\mathscr{F}$, for $\alpha < 0$ or $\alpha > 1$; whereas for $0 < \alpha < 1$, minimum (n, m)-graphs must belong to the family $\mathscr{F}$.

Lemma 3.3. *For $\alpha < 0$ or $\alpha > 1$, a maximum (n, m)-graph G has at least one vertex of degree $n - 1$; whereas for $0 < \alpha < 1$, a minimum (n, m)-graph G has at least one vertex of degree $n - 1$.*

Proof. Here we only consider the case $0 < \alpha < 1$. Let G be a minimum (n, m)-graph, and x_0 be a vertex with maximum degree in G and $d(x_0) = l < n - 1$. Then there is an edge y_1y_2 $(y_1, y_2 \neq x_0)$ satisfying that at least one vertex in $\{y_1, y_2\}$, say y_1, is not adjacent to x_0 (if y_1, y_2 are all not adjacent to x_0, let y_2 be the vertex such that x_0 and y_2 are in the same component of $G - y_1y_2$). Let the connected graph $G' = G - y_1y_2 + x_0y_1$ and $d(y_2) = i \leqslant l$. In other words, G' is obtained from G by replacing the pair (l, i) by $(l + 1, i - 1)$. Then by Lemma 3.1, ${}^0R_\alpha(G') < {}^0R_\alpha(G)$, a contradiction. □

Theorem 3.4. *For $0 < \alpha < 1$, a minimum (n, m)-graph G must be in $\mathscr{F}$; whereas for $\alpha < 0$ and $\alpha > 1$, a maximum (n, m)-graph G must be in $\mathscr{F}$.*

Proof. Here we only consider the case $0 < \alpha < 1$. Suppose G is a minimum (n, m)-graph and so $|V(G)| = n$. We define a sequence $G = G_0, G_1, G_2, \ldots$ of graphs as follows. From Lemma 3.3, we know that $\Delta(G) = n - 1$. Suppose $d_G(x_1) = n - 1$. The graph $G - \{x_1\}$ consists of a connected graph G_1 with no isolated vertices, together with a set J_1 of isolated vertices. If G_1 is the null graph, we are done. Otherwise, let n' be the order of G_1 (note that n' is viewed as a constant here). By Lemma 3.3, we claim that $\Delta(G_1) = |V(G_1)| - 1 = n' - 1$, since G_1 is a minimum $(n', m - n - 1)$-graph. In fact, let $d_1, d_2, \ldots, d_{n'}$ be the degree sequence of G_1, then ${}^0R_\alpha(G_1) = \sum_{i=1}^{n'} d_i^\alpha$ attains minimum if and only if ${}^0R_\alpha(G) = (n - 1)^\alpha + (n - n' - 1)1^\alpha + \sum_{i=1}^{n'} (d_i + 1)^\alpha$ attains minimum.

Suppose that $d_{G_1}(x_2) = |V(G_1)| - 1$. Then the graph $G_1 - \{x_2\}$ consists of a graph G_2 with no isolated vertices, together with a set J_2 of isolated vertices. If G_2 is the null graph then $G = G(d_G(x_1), d_G(x_2))$, and we are done. Otherwise we continue and find a sequence of vertices $\{x_3, x_4, \ldots\}$ and graphs $\{G_3, G_4, \ldots\}$. Eventually, the process terminates with a vertex $x_N \in V(G_{N-1})$ (where $N < n$ is a positive integer) joined to a set J_N of isolated vertices. We then have $G = G(d_G(x_1), d_G(x_2), \ldots, d_G(x_N)) \in \mathscr{F}$. □

Theorem 3.5. *Let $G(n, m)$ be a simple connected graph with n vertices and m edges. If $m = n + k(k - 3)/2 + p$, where $2 \leqslant k \leqslant n - 1$ and $0 \leqslant p \leqslant k - 2$, then for $\alpha \leqslant -1$,*

$$\begin{aligned} {}^0R_\alpha(G(n, m)) &\leqslant {}^0R_\alpha(L^*) \\ &= (n - k - 1) \cdot 1^\alpha + (p + 1)^\alpha + (k - p - 1)(k - 1)^\alpha + p \cdot k^\alpha + (n - 1)^\alpha. \end{aligned} \tag{3.1}$$

4. Proof of Theorem 3.5

Firstly, we introduce some useful lemmas. And we always assume $\alpha \leqslant -1$ in this section. Denote by n_i the number of vertices of degree i.

Lemma 4.1 (Pavlović [16, Lemma 3]). *If $n_1 \neq 0$ in $G(n, m)$, then $n_{n-1} \leqslant 1$. If $n_1 = n_2 = \cdots = n_{i-1} = 0$ and $n_i \neq 0$, then $n_{n-1} \leqslant i$.*

Lemma 4.2 (Pavlović [16, Lemma 4]). *If $n_{n-1} = 1$ and $n_1 = l$ $(l \geqslant 2)$ in $G(n, m)$, then $n_{n-l} = n_{n-l+1} = \cdots = n_{n-3} = n_{n-2} = 0$.*

Lemma 4.3. *Let r, s and t be real numbers such that $0 < r \leqslant s \leqslant t$. Then*

$$(t-r)s^{\alpha} \leqslant (t-s)r^{\alpha} + (s-r)t^{\alpha}$$

and the equality holds only for $s = r$ and t.

Proof. If $s = r$ or $s = t$, it is obvious that equality holds. Denote by $f(s) = (t-s)r^{\alpha} + (s-r)t^{\alpha} - (t-r)s^{\alpha}$. Then $\partial^2 f/\partial s^2 = -\alpha(\alpha-1)(t-r)s^{\alpha-2} < 0$ and the upper inequality follows because the function f is strictly concave. □

Corollary 4.4. *For real number $s > 1$, holds $2s^{\alpha} < (s-1)^{\alpha} + (s+1)^{\alpha}$.*

Then, we will prove that L^* has the maximum ${}^0R_{\alpha}$-value for $\alpha \leqslant -1$ among (n, m)-connected graphs. It means that the maximum (n, m) graph must have $n_1 = n - k - 1$, $n_{p+1} = 1$, $n_{k-1} = k - 1 - p$, $n_k = p$ and $n_{n-1} = 1$.

Theorem 3.5 describes the solution of the following problem (P):

$$\max n_1 \cdot 1^{\alpha} + n_2 \cdot 2^{\alpha} + \cdots + n_{n-1} \cdot (n-1)^{\alpha}$$

under two graph constraints

$$n_1 + n_2 + n_3 + \cdots + n_{n-1} = n, \tag{4.2}$$

$$n_1 + 2n_2 + 3n_3 + \cdots + (n-1)n_{n-1} = 2m. \tag{4.3}$$

It is not difficult to prove the theorem for trees, i.e., $m = n - 1$.

Theorem 4.5. *If $m = n - 1$, the function ${}^0R_{\alpha}$ attains maximum at the star.*

Proof. If $m = n - 1$, then $k = 2$ and $p = 0$. We find n_1 and n_{n-1} from constraints (4.2) and (4.3)

$$n_1 = n - 1 - \left(1 - \frac{1}{n-2}\right) n_2 - \left(1 - \frac{2}{n-2}\right) n_3 - \cdots - \left(1 - \frac{n-3}{n-2}\right) n_{n-2},$$

$$n_{n-1} = 1 - \frac{n_2}{n-2} - \frac{2n_3}{n-2} - \frac{3n_4}{n-2} - \cdots - \frac{(n-3)n_{n-2}}{n-2}.$$

After their substitution into ${}^0R_{\alpha}$, this function becomes

$${}^0R_{\alpha} = n - 1 + (n-1)^{\alpha} + \sum_{j=2}^{n-2} \left(j^{\alpha} - \frac{n-1-j}{n-2} - \frac{j-1}{n-2}(n-1)^{\alpha} \right) n_j.$$

By Lemma 4.3, we have $(n-2)j^{\alpha} \leqslant (n-1-j)1^{\alpha} + (j-1)(n-1)^{\alpha}$ for $1 \leqslant j \leqslant n-1$. We conclude that ${}^0R_{\alpha}$ attains maximum for $n_j = 0$, $j = 2, 3, \ldots, n-2$. Then, $n_1 = n - 1$, $n_2 = n_3 = \cdots = n_{n-2} = 0$, $n_{n-1} = 1$ and $\max_{m=n-1} {}^0R_{\alpha} = n - 1 + (n-1)^{\alpha}$. □

If we want to find extremal graphs for other values of m, we cannot use the same method because the solutions may not correspond to graphs.

Since $m = n + k(k-3)/2 + p$, where $2 \leqslant k \leqslant n-1$ and $0 \leqslant p \leqslant k-2$, we need to consider two cases: (1) $k = n - 1$ and (2) $2 \leqslant k \leqslant n-2$. At first, we will prove the theorem for $k = n - 1$.

Case 1: $k = n - 1$.

Lemma 4.6. *Inequality* (3.1) *holds for the graphs $G(n, m)$, $m = n + k(k-3)/2 + p$, where $k = n - 1$ and $0 \leqslant p \leqslant n - 3$.*

Proof. The number of edges is $m = (n^2 - 3n + 4 + 2p)/2 = (n-1)(n-2)/2 + p + 1$, where $0 \leqslant p \leqslant n-3$. If $p \geqslant 1$, then $n_1 = n_2 = n_3 = \cdots = n_p = 0$ and $n_{p+1} \geqslant 0$. Contrary to this, if $G(n, m)$ would have one vertex of degree p (or less), by deleting one vertex of degree p we get the graph $G'(n-1, m-p)$ (not necessarily connected), which has more edges than the complete graph on $n-1$ vertices. The fact that $n_{p+1}\geqslant 0$ means: $n_{p+1}\neq 0$ or $n_{p+1}=0$, $n_{p+2}\neq 0$ or $n_{p+1}=n_{p+2}=0$, $n_{p+3}\neq 0$ and so on. Denote by $P^{(p,p+j+1)}$ the problem for given p when $n_1=n_2=\cdots=n_p=n_{p+1}=n_{p+2}=\cdots=n_{p+j}=0$, $n_{p+j+1}\neq 0$ and by ${}^0R_\alpha^{(p,p+j+1)}$ the optimal value of ${}^0R_\alpha$ for the problem $P^{(p,p+j+1)}$. The optimal value of ${}^0R_\alpha$ for given $p$is ${}^0R_\alpha^p=\max_{0\leqslant j\leqslant n-p-4}{}^0R_\alpha^{(p,p+j+1)}$. If we have $n_{p+j+1}\neq 0$, then $n_{n-1}\leqslant p+j+1$ (Lemma 4.1).

Let us solve the problem $P^{(p,p+j+1)}$, $0\leqslant p\leqslant n-4$, $0\leqslant j\leqslant n-p-4$. (When $p=n-3$, we have only one graph, which is the complete graph with one edge deleted.)

$$\max n_{p+j+1}(p+j+1)^\alpha+n_{p+j+2}(p+j+2)^\alpha+\cdots+n_{n-1}(n-1)^\alpha$$

under the constraints:

$$n_{p+j+1}+n_{p+j+2}+n_{p+j+3}+\cdots+n_{n-1}=n,$$

$$(p+j+1)n_{p+j+1}+(p+j+2)n_{p+j+2}+\cdots+(n-1)n_{n-1}=n^2-3n+4+2p,$$

$$n_{n-1}=p+j+1-\xi,$$

where $0\leqslant\xi\leqslant j$. Let us solve the system of the latter three equations in n_{n-1}, n_{n-2} and n_{p+j+1}:

$$\begin{aligned}n_{n-2}=&\frac{n^2-n(2p+2j+5)+p^2+2pj+5p+j^2+3j+6}{n-p-j-3}-\frac{n_{p+j+2}}{n-p-j-3}\\&-\frac{2n_{p+j+3}}{n-p-j-3}-\frac{3n_{p+j+4}}{n-p-j-3}\\&-\cdots-\frac{(n-p-j-4)n_{n-3}}{n-p-j-3}+\frac{(n-p-j-2)\xi}{n-p-j-3},\end{aligned}$$

$$\begin{aligned}n_{p+j+1}=&\frac{n-p+j-3}{n-p-j-3}-\left(1-\frac{1}{n-p-j-3}\right)n_{p+j+2}\\&-\left(1-\frac{2}{n-p-j-3}\right)n_{p+j+3}-\left(1-\frac{3}{n-p-j-3}\right)n_{p+j+4}\\&-\cdots-\left(1-\frac{n-p-j-4}{n-p-j-3}\right)n_{n-3}+\left(1-\frac{n-p-j-2}{n-p-j-3}\right)\xi.\end{aligned}$$

After substituting n_{p+j+1}, n_{n-2}, n_{n-1} back into ${}^0R_\alpha$, we have

$$\begin{aligned}{}^0R_\alpha=&\frac{n-p+j-3}{n-p-j-3}(p+j+1)^\alpha+(p+j+1)(n-1)^\alpha\\&+\frac{n^2-n(2p+2j+5)+p^2+2pj+5p+j^2+3j+6}{n-p-j-3}(n-2)^\alpha\\&+\sum_{i=p+j+2}^{n-3}n_i\left(i^\alpha-\frac{n-i-2}{n-p-j-3}(p+j+1)^\alpha-\frac{i-p-j-1}{n-p-j-3}(n-2)^\alpha\right)\\&+\xi\left(-(n-1)^\alpha-\frac{1}{n-p-j-3}(p+j+1)^\alpha+\frac{n-p-j-2}{n-p-j-3}(n-2)^\alpha\right).\end{aligned}$$

We have (because of Lemma 4.3)

$$(n-p-j-3)i^\alpha\leqslant(n-i-2)(p+j+1)^\alpha+(i-p-j-1)(n-2)^\alpha\quad\text{for } p+j+1\leqslant i\leqslant n-2,$$

$$(n-p-j-2)(n-2)^\alpha\leqslant(p+j+1)^\alpha+(n-p-j-3)(n-1)^\alpha.$$

The latter inequality is obtained for $i=n-2$ from the inequality

$$(n-p-j-2)i^{\alpha} \leqslant (n-i-1)(p+j+1)^{\alpha} + (i-p-j-1)(n-1)^{\alpha} \quad \text{for } p+j+1 \leqslant i \leqslant n-1.$$

It means that we will get the maximum value of ${}^0R_{\alpha}$ if we put $n_{p+j+2}=n_{p+j+3}=\cdots=n_{n-3}=\xi=0$ and

$$\begin{aligned}{}^0\tilde{R}_{\alpha}^{(p,p+j+1)} = {} & \frac{n-p+j-3}{n-p-j-3}(p+j+1)^{\alpha} + (p+j+1)(n-1)^{\alpha} \\ & + \frac{n^2-n(2p+2j+5)+p^2+2pj+5p+j^2+3j+6}{n-p-j-3}(n-2)^{\alpha}\end{aligned}$$

for $p=0,1,\ldots,n-4$ and $j=0,1,\ldots,n-p-4$. This solution does not always correspond to a graph (except for $j=0$, ${}^0\tilde{R}_{\alpha}^{(p,p+1)}={}^0R_{\alpha}^{(p,p+1)}$). We put symbol $\sim$ for this solution, but the true graph solution, ${}^0R_{\alpha}^{(p,p+j+1)}$ is less than or equal to ${}^0\tilde{R}_{\alpha}^{(p,p+j+1)}$.

Now we show that ${}^0R_{\alpha}^{(p,p+1)}$ is the maximum value of ${}^0R_{\alpha}$ for a given number p, that is, ${}^0R_{\alpha}^{(p,p+1)}=\max_{0\leqslant j\leqslant n-p-4} {}^0R_{\alpha}^{(p,p+j+1)}$. Since ${}^0R_{\alpha}^{(p,p+j+1)} \leqslant {}^0\tilde{R}_{\alpha}^{(p,p+j+1)}$, it is sufficient to prove that ${}^0R_{\alpha}^{(p,p+1)}=\max_{0\leqslant j\leqslant n-p-4} {}^0\tilde{R}_{\alpha}^{(p,p+j+1)}$. We have to prove the following inequality:

$${}^0\tilde{R}_{\alpha}^{(p,p+j+1)} \leqslant (p+1)^{\alpha} + (n-p-2)(n-2)^{\alpha} + (p+1)(n-1)^{\alpha}. \tag{4.4}$$

We transform inequality (4.4) (for $n-p-j-3 \neq 0$) into (4.5)

$$\begin{aligned} f(j) = {} & (n-p-j-3)(p+1)^{\alpha} - (n-p+j-3)(p+j+1)^{\alpha} \\ & + j(n-p-j-1)(n-2)^{\alpha} - j(n-p-j-3)(n-1)^{\alpha} \geqslant 0. \end{aligned} \tag{4.5}$$

Since $f(0)=f(n-p-3)=0$, we only need to prove $\partial^2 f/\partial j^2 \leqslant 0$. We have

$$\partial^2 f/\partial j^2 = -\alpha(p+j+1)^{\alpha-2}\,(2(p+j+1)+(\alpha-1)(n-p+j-3)) - 2((n-2)^{\alpha}-(n-1)^{\alpha}),$$

and since $-2((n-2)^{\alpha}-(n-1)^{\alpha}) \leqslant 0$, we have to prove

$$2(p+j+1)+(\alpha-1)(n-p+j-3) = (n-p+j-3)\alpha - n + 3p + j + 5 \leqslant 0. \tag{4.6}$$

Since $0 \leqslant p \leqslant n-4$ and $0 \leqslant j \leqslant n-p-4$, we have $0 \leqslant p+j \leqslant n-4$ and

$$\begin{aligned} n-3p-j-5 &= n-2p-(p+j)-5 \geqslant n-2p-(n-4)-5 \\ &= -2p-1 \geqslant -2(n-4)-1 = -2n+7, \end{aligned}$$

$$n-p+j-3 \leqslant n-p+(n-p-4)-3 = 2n-7-2p \leqslant 2n-7.$$

So we have

$$\frac{n-3p-j-5}{n-p+j-3} \geqslant \frac{-2n+7}{2n-7} = -1 \geqslant \alpha.$$

Then inequality (4.6) holds for $\alpha \leqslant -1$.

We have proved that the maximum value of ${}^0R_{\alpha}$ for a given number p is ${}^0R_{\alpha}^{(p,p+1)}$

$${}^0R_{\alpha}^{(p,p+1)} = (p+1)^{\alpha} + (n-p-2)(n-2)^{\alpha} + (p+1)(n-1)^{\alpha}$$

for $p=0,1,\ldots,n-4$. This value is attained at a graph which has $n_{n-1}=p+1$, $n_{n-2}=n-p-2$ and $n_{p+1}=1$.

Case 2: $2 \leqslant k \leqslant n-2$.

We have proved the theorem for $k=n-1$, in which case $m \geqslant (n-1)(n-2)/2+1$. It remains to prove the theorem for $m \leqslant (n^2-3n+2)/2$. Denote by $G^*=G^*(n,m)$ the graph at which ${}^0R_{\alpha}$ attains maximum. □

Lemma 4.7. *If a maximum graph G^* has r $(r \leqslant n-3)$ vertices of degree $n-1$, then the minimum degree of G^* is r.*

Proof. If not, let l be the minimum degree of G^*, and $l \geqslant r+1$. Let u be a vertex of degree l. Let v be a neighbor vertex of u such that $d(v) < n-1$. Then there exists a vertex w with degree j $(l \leqslant j < n-1)$ such that $vw \notin E(G^*)$. Denote by G' a graph obtained from G^* by deleting the edge uv and adding a new edge vw. Then by Lemma 3.1, we have ${}^0R_\alpha(G') > {}^0R_\alpha(G^*)$, a contradiction. □

Lemma 4.8. *If* $m \leqslant (n^2-3n+2)/2$, *then* $n_1(G^*) \neq 0$, *for any maximum graph* G^*.

Proof. Suppose to the contrary, $n_1(G^*) = 0$. Without loss of generality, we can suppose that the minimum degree of G^* is r, i.e., $n_1 = n_2 = \cdots = n_{r-1} = 0$ and $n_r \neq 0$ for $r \geqslant 2$. Then G^* has r vertices of degree $n-1$. For otherwise, if G^* has $k \neq r$ vertices of degree $n-1$, by Lemma 4.7 we have that the minimum degree of G^* is $k \neq r$. Let u be a vertex of degree r, then u is joined with all vertices $w_1, w_2, \ldots, w_r$ of maximum degree $n-1$.

Denote by $S(G^*)$ the subgraph induced by $G^* \backslash \{u, w_1, w_2, \ldots, w_r\}$, and $K(G^*)$ the complete graph on $V(S(G^*))$. Then

$$\begin{aligned} |E(K(G^*))| - |E(S(G^*))| &= \binom{n-r-1}{2} - \left(m - r(n-r) - \binom{r}{2}\right) \\ &\geqslant \binom{n-r-1}{2} - \frac{n^2-3n+2}{2} + r(n-r) + \binom{r}{2} \\ &= r. \end{aligned}$$

It means that we can add at least $r-1$ edges in $S(G^*)$, and after that, these vertices do not still form a complete graph.

For $r \geqslant 2$, denote by G' a simple connected graph obtained from G^* when we delete $r-1$ edges between vertex u and vertices $w_2, \ldots, w_r$ and add $r-1$ new edges among $n-r-1$ vertices between $r-1$ pairs of vertices: v_1 (degree j_1) and v_1' (degree j_1'), v_2 (degree j_2) and v_2' (degree j_2'), $\ldots$, v_{r-1} (degree j_{r-1}) and v_{r-1}' (degree j_{r-1}'), and these vertices are not necessarily distinct.

If all these vertices are distinct, then the degree of v_i (v_i') $(i = 1, 2, \ldots, r-1)$, increases by 1. We have

$$\begin{aligned} {}^0R_\alpha(G') - {}^0R_\alpha(G^*) &= 1 - r^\alpha + (r-1)(n-2)^\alpha - (r-1)(n-1)^\alpha + (j_1+1)^\alpha - j_1^\alpha \\ &\quad + (j_1'+1)^\alpha - (j_1')^\alpha + (j_2+1)^\alpha - j_2^\alpha + (j_2'+1)^\alpha - (j_2')^\alpha + \cdots \\ &\quad + (j_{r-1}+1)^\alpha - j_{r-1}^\alpha + (j_{r-1}'+1)^\alpha - (j_{r-1}')^\alpha \\ &> 1 - r^\alpha + 2(r-1)((r+1)^\alpha - r^\alpha) \end{aligned}$$

the last inequality holds because $(j+1)^\alpha - j^\alpha$ is an increasing function.

Moreover, there may exist some vertices used more than once. Suppose the degree of v_i (v_i') increases by x_i (x_i') $(i = 1, 2, \ldots, r-1)$, then for $1 \leqslant i \leqslant r-1$, $x_i, x_i' \geqslant 0$, we have $\sum_{i=1}^{r-1} x_i = r-1$, $\sum_{i=1}^{r-1} x_i' = r-1$ and

$$((j+x)^\alpha - j^\alpha) - x((r+1)^\alpha - r^\alpha) \geqslant 0 \quad \text{for } x \geqslant 0. \tag{4.7}$$

In fact, if $j \geqslant r+1$, then $((j+x)^\alpha - j^\alpha) - x((r+1)^\alpha - r^\alpha) = \alpha x(\xi_1^{\alpha-1} - \xi_2^{\alpha-1}) \geqslant 0$, where $\xi_1 \in (j, j+x)$, $\xi_2 \in (r, r+1)$.

And if $j = r$, we need to prove

$$((r+x)^\alpha - r^\alpha) - x((r+1)^\alpha - r^\alpha) \geqslant 0.$$

We proceed by induction on x. When $x = 0$, the inequality holds. Suppose the inequality holds for $x \geqslant 0$, and consider the case of $x+1$. By induction hypothesis,

$$\begin{aligned} (r+x+1)^\alpha - r^\alpha &= ((r+x)^\alpha - r^\alpha) + ((r+x+1)^\alpha - (r+x)^\alpha) \\ &\geqslant x((r+1)^\alpha - r^\alpha) + ((r+x+1)^\alpha - (r+x)^\alpha) \\ &\geqslant x((r+1)^\alpha - r^\alpha) + ((r+1)^\alpha - r^\alpha) \\ &= (x+1)((r+1)^\alpha - r^\alpha). \end{aligned}$$

Thus, we have proved the inequality (4.7).

So, we have

$$\begin{aligned}{}^0R_\alpha(G') - {}^0R_\alpha(G^*) &= 1 - r^\alpha + (r-1)(n-2)^\alpha - (r-1)(n-1)^\alpha \\ &\quad + (j_1+x_1)^\alpha - j_1^\alpha + (j_1'+x_1')^\alpha - (j_1')^\alpha + (j_2+x_2)^\alpha - j_2^\alpha \\ &\quad + (j_2'+x_2')^\alpha - (j_2')^\alpha + \cdots + (j_{r-1}+x_{r-1})^\alpha - j_{r-1}^\alpha \\ &\quad + (j_{r-1}'+x_{r-1}')^\alpha - (j_{r-1}')^\alpha \\ &> 1 - r^\alpha + 2(r-1)((r+1)^\alpha - r^\alpha) \\ &= 1 - r^\alpha + 2\alpha(r-1)\xi^{\alpha-1} \\ &> 1 - r^\alpha + 2\alpha(r-1)r^{\alpha-1} \\ &= 1 - (r - 2\alpha(r-1))r^{\alpha-1} \geqslant 0,\end{aligned}$$

where $\xi \in (r, r+1)$.

In order to prove the last inequality, we only need to prove

$$f(\alpha) = r^{1-\alpha} + 2\alpha(r-1) - r \geqslant 0 \quad \text{for } r \geqslant 2.$$

But $f'(\alpha) = -r^{1-\alpha}\ln r + 2(r-1) < 0$, for $r \geqslant 2$. This implies $f(\alpha) \geqslant f(-1) = r^2 - 3r + 2 = (r-1)(r-2) \geqslant 0$ for $r \geqslant 2$, and then $f(\alpha) \geqslant f(-1) = 0$ for $\alpha \leqslant -1$. □

Hence, we only need to consider maximum graphs which have $n_1 \neq 0$, for $2 \leqslant k \leqslant n-2$. Then $n_{n-1} = 1$ (Lemmas 4.1 and 3.3) and all vertices of degree 1 must be adjacent to this unique vertex of degree $n-1$.

When $n_{n-1} = 1$ and $n_1 = l$, instead of problem (P) we can consider the following problem (P^l):

$$\max l \cdot 1^\alpha + n_2 \cdot 2^\alpha + \cdots + n_{n-l-1}(n-l-1)^\alpha + (n-1)^\alpha$$

under the constraints:

$$n_2 + n_3 + n_4 + \cdots + n_{n-l-1} = n - 1 - l, \tag{4.8}$$

$$n_2 + 2n_3 + 3n_4 + \cdots + (n-l-2)n_{n-l-1} = 2(m-n+1). \tag{4.9}$$

The proof of following lemma is based on mathematical induction. It is easy to check that the theorem is true for $n = 5$ and $4 \leqslant m \leqslant 10$. We will suppose that the theorem is true for every graph $G(i, j)$, such that $5 \leqslant i \leqslant n-1$ and $i - 1 \leqslant j \leqslant \binom{i}{2}$. We have to prove the theorem for graphs $G(n, m)$, such that $n - 1 \leqslant m \leqslant \binom{n}{2}$. The case $m = n-1$ was already considered above, and the cases $m = \binom{n}{2}$ and $\binom{n}{2} - 1$ will not be considered because each corresponds to a unique graph.

Lemma 4.9. *Inequality* (3.1) *holds for all graphs* $G(n, m)$ *with* $n_{n-1} = 1$ *and* $n_1 = l$ $(l \geqslant 1)$, *for* $2 \leqslant k \leqslant n-2$.

Proof. Inequality (3.1) will be valid for all graphs $G(n, m)$ with $n_{n-1} = 1$ and $n_1 = l$, if the following inequality holds:

$$\begin{aligned}&l + n_2 \cdot 2^\alpha + n_3 \cdot 3^\alpha + \cdots + n_{n-l-1}(n-l-1)^\alpha + (n-1)^\alpha \\ &\quad \leqslant n - k - 1 + (p+1)^\alpha + (k-p-1)(k-1)^\alpha + p \cdot k^\alpha + (n-1)^\alpha\end{aligned} \tag{4.10}$$

under constraints (4.8) and (4.9).

We first prove (4.10) for $l \geqslant 2$. Since $n_1 = l$, by Lemma 4.2 we have $n_{n-l} = n_{n-l+1} = \cdots = n_{n-2} = 0$. Consider the graph $G'(n-1, m-1)$, which is obtained from $G(n, m)$, when we delete one vertex of degree 1. The graph $G'(n-1, m-1)$ has $n_1' = l - 1$ and one vertex of degree $n-2$ (because the other vertices can have degree at most $n-1-l$), and $n_i' = n_i$ for $i = 2, \ldots, n-3$. Then $n_{n-l}' = n_{n-l+1}' = \cdots = n_{n-3}' = 0$ (because $n - 1 - (l-1) = n - l$)

and the same constraints (4.8) and (4.9) hold. Since $G'(n-1, m-1)$ has $n-1$ vertices and $n-1+k(k-3)/2+p$ edges, it satisfies the inductive hypothesis, and so,

$$\begin{aligned} & n_2 \cdot 2^{\alpha} + n_3 \cdot 3^{\alpha} + \cdots + n_{n-l-1}(n-l-1)^{\alpha} \\ & \quad = n_2' \cdot 2^{\alpha} + n_3' \cdot 3^{\alpha} + \cdots + n_{n-l-1}'(n-l-1)^{\alpha} \\ & \quad \leqslant n-k-1-l+(p+1)^{\alpha}+(k-p-1)(k-1)^{\alpha}+p \cdot k^{\alpha} \end{aligned} \tag{4.11}$$

for every $2 \leqslant k \leqslant n-2$ and $0 \leqslant p \leqslant k-2$. Inequality (4.11) is equivalent to (4.10), which is now proved because the constraints are the same.

Now we show that (4.10) holds for $l=1$, that is, the graph G' has no vertex of degree one. We have $n_i' = n_i$ for $i = 2, \ldots, n-3$ and $n_{n-2}' = n_{n-2}+1$. By the inductive hypothesis for the graph G' holds

$$\begin{aligned} & n_2 \cdot 2^{\alpha} + n_3 \cdot 3^{\alpha} + \cdots + (n_{n-2}+1)(n-2)^{\alpha} \\ & \quad = n_2' \cdot 2^{\alpha} + n_3' \cdot 3^{\alpha} + \cdots + n_{n-2}'(n-2)^{\alpha} \\ & \quad \leqslant (n-1)-k-1+(p+1)^{\alpha}+(k-p-1)(k-1)^{\alpha}+p \cdot k^{\alpha}+(n-2)^{\alpha} \end{aligned} \tag{4.12}$$

under the constraints

$$\begin{aligned} & n_2' + n_3' + n_4' + \cdots + n_{n-2}' = n-1, \\ & 2n_2' + 3n_3' + 3n_4' + \cdots + (n-2)n_{n-2}' = 2(m-1). \end{aligned} \tag{4.13}$$

Namely, it holds

$$\begin{aligned} & n_2 \cdot 2^{\alpha} + n_3 \cdot 3^{\alpha} + \cdots + n_{n-3}(n-3)^{\alpha} + n_{n-2}(n-2)^{\alpha} \\ & \quad \leqslant n-k-2+(p+1)^{\alpha}+(k-p-1)(k-1)^{\alpha}+p \cdot k^{\alpha} \end{aligned} \tag{4.14}$$

under the constraints

$$\begin{aligned} & n_2 + n_3 + \cdots + n_{n-3} + n_{n-2} = n-2, \\ & n_2 + 2n_3 + \cdots + (n-4)n_{n-3} + (n-3)n_{n-2} = 2(m-n+1). \end{aligned} \tag{4.15}$$

Equalities (4.15) are just the constraints (4.8) and (4.9), and inequality (4.14) is equivalent to inequality (4.10) for $l=1$.

Finally, after considering all cases we proved the theorem. □

5. Concluding remarks

In this paper, we discuss general connected (n, m)-graphs with the extremal value of zeroth-order general Randić index. We use the following table to summarize our main results. For α in some intervals, it remains to determine exactly which graphs in the family $\mathscr{F}$ are extremal.

	$\alpha < 0$ or $\alpha > 1$		$0 < \alpha < 1$
Minimum graph	Nearly regular graph		in $\mathscr{F}$
Maximum graph	$\alpha \leqslant -1$	$\alpha > -1$	Nearly regular graph
	L^*	in $\mathscr{F}$	

Acknowledgments

The authors are very grateful to the anonymous referees for their valuable suggestions, corrections and comments that helped to improve the original manuscript.

References

[1] D. Amic, D. Beslo, B. Lucic, S. Nikolic, N. Trinajstic, The vertex-connectivity index revisited, J. Chem. Inf. Comput. Sci. 38 (1998) 819–822.
[2] B. Bollobás, P. Erdös, Graphs of extremal weights, Ars Combin. 50 (1998) 225–233.
[3] B. Bollobás, P. Erdös, A. Sarkar, Extremal graphs for weights, Discrete Math. 200 (1999) 5–19.
[4] J.A. Bondy, U.S.R. Murty, Graph Theory with Applications, Macmillan Press Ltd., London, 1976.
[5] G. Caporossi, I. Gutman, P. Hansen, L. Pavlović, Graphs with maximum connectivity index, Comput. Biol. Chem. 27 (2003) 85–90.
[6] Y. Hu, X. Li, Y. Shi, T. Xu, I. Gutman, On molecular graphs with smallest and greatest zeroth-order general Randic index, MATCH Commun. Math. Comput. Chem. 54 (2) (2005) 425–434.
[7] Y. Hu, X. Li, Y. Yuan, Trees with minimum general Randić index, MATCH Commun. Math. Comput. Chem. 52 (2004) 119–128.
[8] Y. Hu, X. Li, Y. Yuan, Trees with maximum general Randić index, MATCH Commun. Math. Comput. Chem. 52 (2004) 129–146.
[9] L.B. Kier, L.H. Hall, Molecular Connectivity in Chemistry and Drug Research, Academic Press, New York, 1976.
[10] L.B. Kier, L.H. Hall, The nature of structure-activity relationships and their relation to molecular connectivity, European J. Med. Chem. 12 (1977) 307–312.
[11] R. Lang, X. Li, S. Zhang, Inverse problem for Zagreb index of molecular graphs, Appl. Math. J. Chinese Univ. Ser. A 18 (2003) 487–493 (in Chinese).
[12] X. Li, I. Gutman, Mathematical Aspects of Randić-Type Molecular Structure Descriptors, Mathematical Chemistry Monographs No. 1, Kragujevac, 2006.
[13] X. Li, Y. Yang, Sharp bounds for the general Randić index, MATCH Commun. Math. Comput. Chem. 51 (2004) 155–166.
[14] X. Li, H. Zhao, Trees with the first three smallest and largest generalized topological indices, MATCH Commun. Math. Comput. Chem. 50 (2004) 57–62.
[15] X. Li, J. Zheng, A unified approach to the extremal trees for different indices, MATCH Commun. Math. Comput. Chem. 54 (1) (2005) 195–208.
[16] L. Pavlović, Maximal value of the zeroth-order Randić index, Discrete Appl. Math. 127 (2003) 615–626.
[17] M. Randić, On characterization of molecular branching, J. Amer. Chem. Soc. 97 (1975) 6609–6615.