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(n, m)-Graphs with Maximum Zeroth-Order General Randić Index for $\alpha \in (-1, 0)$ *

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Abstract

Given a graph $G = (V, E)$ and an arbitrary real number α, the zeroth-order general Randić index of the graph G is defined as ${}^0R_\alpha(G) = \sum_{u \in V(G)} d(u)^\alpha$, where the summation goes over all vertices of G and $d(u)$ denotes the degree of u in G. In this paper, we characterize the simple connected (n, m)-graphs with the maximum zeroth-order general Randić index for $\alpha \in (-1, 0)$, which was left unsolved in our early paper published in Discrete Appl. Math.

1 Introduction

It is well known that Randić index was introduced by Randić [11] 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 B. Bollobás and P. Erdös [2], and D. Amic *et al.* [1], independently, in 1998. Then it has been extensively studied by both mathematicians and theoretical chemists. For a survey of results, we refer to [6] and [7].

The zeroth-order Randić index defined by Kier and Hall [5] is ${}^0R(G) = \sum_{u \in V(G)} d(u)^{-\frac{1}{2}}$. Later Li and Zheng in [8] defined the zeroth-order general Randić index ${}^0R_\alpha(G)$ of a graph

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G as ${}^0R_\alpha(G) = \sum_{v\in V(G)} d(u)^\alpha$ for general real number α. Pavlović [9] determined the graph with the maximum value of ${}^0R(G)$. In [4], Hu et. al. 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 [3], Hu et. al. characterized the simple connected (n,m)-graphs with maximum zeroth-order general Randić index for $\alpha \le -1$ and $0 < \alpha < 1$. In this paper we also investigate the zeroth-order general Randić index for general simple connected (n,m)-graphs. Based on the proof and the results of [3], we characterize the simple connected (n,m)-graphs with maximum zeroth-order general Randić index for $\alpha \in (-1,0)$, which was left unsolved in [3].

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 [3, 9]) 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 3 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 4 vertices. For $m = n+2, n+3, \ldots$, we continue to add edges in this way until we arrive at a complete graph. Then we have $m = n + k(k-3)/2 + p$, where k $(2 \le k \le n-1)$ denotes the number of vertices in the clique, and p denotes the number of vertices with degree k. It is easy to see k and p satisfy that

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

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

2 Main results

In this paper, we will prove the following theorem.

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

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

In fact, the proof of this theorem is based on the proof of Theorem 3.5 of [3], which gave the same extremal graph L^* with the maximum zeroth-order general Randić index for $\alpha \le -1$. All the proof of Theorem 3.5 in [3] for $\alpha < 0$ is valid except for the inequality (4.5) and Lemma 4.8. Thus we only need to prove the following two lemmas for $\alpha \in (-1,0)$. In [3], the authors proved inequality (4.5) for $\alpha \leq -1$. However, there are some errors in their proof, here we will give a corrected proof for $\alpha < 0$. In Lemma 1, the inequality considered is inequality (4.5) of [3].

Lemma 1 *Let n, p, j are integers. For $\alpha < 0$,*

$$\begin{aligned} f(p,j) &= (n-p-j-3)(p+1)^{\alpha} - (n-p+j-3)(p+j+1)^{\alpha} \\ &\quad + j(n-p-j-1)(n-2)^{\alpha} - j(n-p-j-3)(n-1)^{\alpha} \geq 0, \end{aligned}$$

where $0 \leq p \leq n-4$ and $0 \leq j \leq n-p-4$.

Proof. In the following, we only consider $1 \leq j \leq n-p-4$, since $f(p,0) = 0$. Firstly,

$$\begin{aligned} \frac{\partial f(p,j)}{\partial p} &= -(p+1)^{\alpha} + \alpha(n-p-j-3)(p+1)^{\alpha-1} + (p+j+1)^{\alpha} \\ &\quad -\alpha(n-p+j-3)(p+j+1)^{\alpha-1} - j(n-2)^{\alpha} + j(n-1)^{\alpha}. \end{aligned}$$

Since $\alpha(\alpha-1)(n-p-j-3)((p+1)^{\alpha-2} - (p+j+1)^{\alpha-2}) \geq 0$ for $\alpha < 0$, we have

$$\begin{aligned} \frac{\partial^2 f(p,j)}{\partial p^2} &= -2\alpha(p+1)^{\alpha-1} + 2\alpha(p+j+1)^{\alpha-1} + \alpha(\alpha-1)(n-p-j-3)(p+1)^{\alpha-2} \\ &\quad -\alpha(\alpha-1)(n-p+j-3)(p+j+1)^{\alpha-2} \\ &\geq -2\alpha\left((p+1)^{\alpha-1} - (p+j+1)^{\alpha-1} + (\alpha-1)j(p+j+1)^{\alpha-2}\right) \\ &= -2j\alpha(\alpha-1)\left(-\xi^{\alpha-2} + (p+j+1)^{\alpha-2}\right) \geq 0, \end{aligned}$$

where $\xi \in (p+1, p+j+1)$. Since $p \leq n-j-3$,

$$\frac{\partial f(p,j)}{\partial p} \leq -(n-j-2)^{\alpha} + (n-2)^{\alpha} - 2j\alpha(n-2)^{\alpha-1} - j((n-2)^{\alpha} - (n-1)^{\alpha}).$$

Define the function $h(j) = -(n-j-2)^{\alpha} + (n-2)^{\alpha} - 2j\alpha(n-2)^{\alpha-1} - j((n-2)^{\alpha} - (n-1)^{\alpha})$. Since $\partial^2 h(j)/\partial j^2 = -\alpha(\alpha-1)(n-j-2)^{\alpha-2} \leq 0$ and $j \geq 1$, we have

$$\begin{aligned} \frac{\partial h(j)}{\partial j} &= \alpha(n-j-2)^{\alpha-1} - 2\alpha(n-2)^{\alpha-1} - ((n-2)^{\alpha} - (n-1)^{\alpha}) \\ &\leq \alpha(n-3)^{\alpha-1} - 2\alpha(n-2)^{\alpha-1} - ((n-2)^{\alpha} - (n-1)^{\alpha}) \\ &\leq \alpha[(n-1)^{\alpha-1} + (n-3)^{\alpha-1} - 2(n-2)^{\alpha-1}] - ((n-2)^{\alpha} - (n-1)^{\alpha}) - \alpha(n-1)^{\alpha-1} \\ &\leq \alpha\eta^{\alpha-1} - \alpha(n-1)^{\alpha-1} \leq 0, \end{aligned}$$

where $\eta \in (n-2, n-1)$. Thus, $\frac{\partial f(p,j)}{\partial p} \leq h(j) \leq h(1)$. By Taylor Expansion, we have

$$\begin{aligned} (n-1)^{\alpha} &= (n-2)^{\alpha} + \alpha(n-2)^{\alpha-1} + \frac{\alpha(\alpha-1)}{2!}(n-2+\xi_1)^{\alpha-2} \\ (n-3)^{\alpha} &= (n-2)^{\alpha} - \alpha(n-2)^{\alpha-1} + \frac{\alpha(\alpha-1)}{2!}(n-2-\xi_2)^{\alpha-2}, \end{aligned}$$

where $0 < \xi_1 < 1$ and $0 < \xi_2 < 1$.

Since

$$\begin{aligned} h(1) &= (n-1)^\alpha - (n-3)^\alpha - 2\alpha(n-2)^{\alpha-1} \\ &= (n-2)^\alpha + \alpha(n-2)^{\alpha-1} + \frac{\alpha(\alpha-1)}{2}(n-2+\xi_1)^{\alpha-2} \\ &\quad - \left((n-2)^\alpha - \alpha(n-2)^{\alpha-1} + \frac{\alpha(\alpha-1)}{2}(n-2-\xi_2)^{\alpha-2}\right) - 2\alpha(n-2)^{\alpha-1} \\ &= \frac{\alpha(\alpha-1)}{2}\left((n-2+\xi_1)^{\alpha-2} - (n-2-\xi_2)^{\alpha-2}\right) \leq 0. \end{aligned}$$

Then $f(p,j) \geq f(n-j-3,j) = 0$. ∎

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

Proof. Firstly, we use the same method as the proof of Lemma 4.8 in [3]. Suppose $n_1(G^*) = 0$ for some maximum graph G^*. Without loss of generality, suppose the minimum degree of G^* is r, i.e., $n_1 = n_2 = \cdots = n_{r-1} = 0$ and $n_r \neq 0$ for $r \geq 2$. Then G^* has r vertices of degree $n-1$. Let u be the vertex of degree r, then u is adjacent to all vertices $w_1, w_2, \ldots, w_r$ with 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 $|E(K(G^*))| - |E(S(G^*))| \geq r$. 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 $r \geq 2$, 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 (j_2) and v_2' (j_2'), …, v_{r-1} (j_{r-1}) and v_{r-1}' (j_{r-1}'), and these vertices are not necessarily distinct.

Then by the similarly discussion as in [3], we have

$${}^0R_\alpha(G') - {}^0R_\alpha(G^*) > 1 - r^\alpha + 2(r-1)((r+1)^\alpha - r^\alpha) > 1 - (r - 2\alpha(r-1))r^{\alpha-1}.$$

Now we will prove ${}^0R_\alpha(G') - {}^0R_\alpha(G^*) > 0$ for $\alpha \in (-1,0)$ and $r \geq 4$. Let $f(\alpha) = r^{1-\alpha} + 2\alpha(r-1) - r$ for $r \geq 5$. By some calculations, we have $f'(\alpha) = -r^{1-\alpha}\ln r + 2(r-1)$ and $f''(\alpha) = (\ln r)^2 r^{1-\alpha}$. Since $f''(\alpha) > 0$, $f'(\alpha) < f'(0) = -r\ln r + 2r - 2$. Set $g(r) = -r\ln r + 2r - 2$, we have $g'(r) = 1 - \ln r < 0$ for $r \geq 5$. So $f'(\alpha) < f'(0) = g(r) < g(5) = 8 - 5\ln 5 < 0$. Therefore, $f(\alpha) > f(0) = 0$, i.e., ${}^0R_\alpha(G') - {}^0R_\alpha(G^*) > 0$ for $\alpha \in (-1,0)$ and $r \geq 5$.

For $r = 4$, we note

$${}^0R_\alpha(G') - {}^0R_\alpha(G^*) > 1 - r^\alpha + 2(r-1)((r+1)^\alpha - r^\alpha) = 6 \cdot 5^\alpha - 7 \cdot 4^\alpha + 1.$$

Let $f_1(\alpha) = 6 \cdot 5^\alpha - 7 \cdot 4^\alpha + 1$, then $f_1'(\alpha) = 6 \ln 5 \cdot 5^\alpha - 7 \ln 4 \cdot 4^\alpha < (6 \ln 5 - 7 \ln 4) 4^\alpha < 0$. We have $f_1(\alpha) > f_1(0) = 0$, i.e., ${}^0R_\alpha(G') - {}^0R_\alpha(G^*) > 0$ for $\alpha \in (-1, 0)$ and $r = 4$.

Suppose $n \geq 8$. For $r = 2$ and $r = 3$, we will construct another new graph G'' from G^*, respectively. Note that $(x+1)^\alpha - x^\alpha$ is an increasing function for $\alpha < 0$.

Case 1. $r = 2$

In this case the maximum graph G^* has only two vertices with degree $n-1$, denoted by w_1 and w_2. Note that $|E(K(G^*))| - |E(S(G^*))| \geq r = 2$. We consider the number of vertices with degree 2, i.e., the value of n_2.

Subcase 1.1. $n_2 = 1$

Let u be the vertex of degree 2, then u is adjacent to w_1, w_2. Since $|E(K(G^*))| - |E(S(G^*))| \geq 2$, it means that we can add at least 1 edges in $S(G^*)$, and after that, these vertices do not still form a complete graph. Let v and v' be two nonadjacent vertices in G^* with degree $j \geq 3$ and $j' \geq 3$, respectively. Construct a new graph $G'' = G^* - uw_1 + vv'$, then we have

$$
\begin{aligned}
{}^0R_\alpha(G'') - {}^0R_\alpha(G^*) &= 1 + (j+1)^\alpha + (j'+1)^\alpha + (n-2)^\alpha - j^\alpha - j'^\alpha - (n-1)^\alpha - 2^\alpha \\
&> 1 + 2 \cdot 4^\alpha - 2^\alpha - 2 \cdot 3^\alpha = (1 - 2^\alpha)^2 + (4^\alpha - 3^\alpha) - (3^\alpha - 2^\alpha) > 0,
\end{aligned}
$$

a contradiction.

Subcase 1.2. $2 \leq n_2 \leq n-3$

Let $u_1, u_2, \ldots, u_{n_2}$ be the vertices of degree 2, then u_i is adjacent to w_1, w_2 for $1 \leq i \leq n_2$. In this subcase, $G^* \setminus \{w_1, w_2, u_1, u_2, \ldots, u_{n_2}\} \neq \emptyset$, choose a vertex $v \in G^* \setminus \{w_1, w_2, u_1, u_2, \ldots, u_{n_2}\}$, note that $vu_i \notin E(G^*)$ for $1 \leq i \leq n_2$. Let $d(v) = j$ $(j \geq 3)$. Construct a new graph $G'' = G^* - u_1w_1 + u_2v$, then we have

$$
\begin{aligned}
{}^0R_\alpha(G'') - {}^0R_\alpha(G^*) &= 1 + 3^\alpha + (j+1)^\alpha + (n-2)^\alpha - j^\alpha - 2 \cdot 2^\alpha - (n-1)^\alpha \\
&> 1 + 3^\alpha - 2 \cdot 2^\alpha + 4^\alpha - 3^\alpha = (1 - 2^\alpha)^2 > 0,
\end{aligned}
$$

a contradiction.

Subcase 1.3. $n_2 = n-2$

Let $u_1, u_2, \ldots, u_{n-2}$ be the vertices of degree 2, then u_i is adjacent to w_1, w_2 for $1 \leq i \leq n-2$. Since $n \geq 8$, $n_2 \geq 6$. Construct a new graph $G'' = G^* - u_1w_1 - u_2w_1 - u_3w_1 + u_4u_5 + u_5u_6 + u_4u_6$, then we have

$$
{}^0R_\alpha(G'') - {}^0R_\alpha(G^*) = 3 + 3 \cdot 4^\alpha + (n-4)^\alpha - 6 \cdot 2^\alpha - (n-1)^\alpha > 3(1 - 2^\alpha)^2 > 0,
$$

a contradiction.

Case 2. $r = 3$

In this case the maximum graph G^* has only three vertices with degree $n-1$, denoted by w_1, w_2 and w_3. Note that $|E(K(G^*))| - |E(S(G^*))| \geq r = 3$. Similarly, we consider the number of vertices with degree 3, i.e., the value of n_3.

Subcase 2.1. $n_3 = 1$

Let u be the vertex of degree 3, then u is adjacent to w_1, w_2, w_3. Since $|E(K(G^*))| - |E(S(G^*))| \geq 3$, it means that we can add at least 2 edges in $S(G^*)$, and after that, these vertices do not still form a complete graph. Let v_1 and v_1', v_2 and v_2' be two pair of nonadjacent vertices in G^* with degrees $j_1 \geq 4$ and $j_1' \geq 4$, $j_2 \geq 4$ and $j_2' \geq 4$, respectively. Note that these four vertices are not necessarily distinct.

If all these four vertices are distinct, we construct a new graph $G'' = G^* - uw_1 - uw_2 + v_1v_1' + v_2v_2'$, then we have

$$\begin{aligned} & {}^0R_\alpha(G'') - {}^0R_\alpha(G^*) \\ = \;& 1 + \sum_{i=1}^{2} ((j_i+1)^\alpha - j_i^\alpha) + \sum_{i=1}^{2} ((j_i'+1)^\alpha - j_i'^\alpha) + 2(n-2)^\alpha - 3^\alpha - 2(n-1)^\alpha \\ > \;& 1 - 3^\alpha + 4(5^\alpha - 4^\alpha). \end{aligned}$$

Let $f_2(\alpha) = 1 - 3^\alpha + 4(5^\alpha - 4^\alpha)$. Since

$$f_2'(\alpha) = -\ln 3 \cdot 3^\alpha + 4\ln 5 \cdot 5^\alpha - 4\ln 4 \cdot 4^\alpha < (-\ln 3 + 4\ln 5 - 4\ln 4)4^\alpha < 0,$$

we have $f_2(\alpha) > f_2(0) = 0$, i.e., ${}^0R_\alpha(G'') - {}^0R_\alpha(G^*) > 0$, a contradiction.

Otherwise, without loss of generality, suppose v_1' and v_2' are the same vertex, denoted by v with degree $j \geq 4$. We construct a new graph $G'' = G^* - uw_1 - uw_2 + v_1v + v_2v$, then we have

$$\begin{aligned} & {}^0R_\alpha(G'') - {}^0R_\alpha(G^*) \\ = \;& 1 + \sum_{i=1}^{2} ((j_i+1)^\alpha - j_i^\alpha) + (j+2)^\alpha - j^\alpha + 2(n-2)^\alpha - 3^\alpha - 2(n-1)^\alpha \\ > \;& 1 + 2(5^\alpha - 4^\alpha) + 6^\alpha - 4^\alpha - 3^\alpha = 1 + 2 \cdot 5^\alpha + 6^\alpha - 3^\alpha - 3 \cdot 4^\alpha. \end{aligned}$$

Let $f_3(\alpha) = 1 + 2 \cdot 5^\alpha + 6^\alpha - 3^\alpha - 3 \cdot 4^\alpha$. Since

$$f_3'(\alpha) = 2\ln 5 \cdot 5^\alpha + \ln 6 \cdot 6^\alpha - \ln 3 \cdot 3^\alpha - 3\ln 4 \cdot 4^\alpha < (2\ln 5 + \ln 6 - \ln 3 - 3\ln 4)5^\alpha < 0,$$

we have $f_3(\alpha) > f_3(0) = 0$, i.e., ${}^0R_\alpha(G'') - {}^0R_\alpha(G^*) > 0$, a contradiction.

Subcase 2.2. $2 \le n_3 \le n-5$

Let $u_1, u_2, \ldots, u_{n_3}$ be the vertices of degree 3, then u_i is adjacent to w_1, w_2, w_3 for $1 \le i \le n_3$. In this subcase, $|G^* \setminus \{w_1, w_2, w_3, u_1, u_2, \ldots, u_{n_3}\}| \ge 2$, choose two vertices $v, v' \in G^* \setminus \{w_1, w_2, u_1, u_2, \ldots, u_{n_2}\}$. Let $d(v) = j$ $(j \ge 4)$ and $d(v') = j'$ $(j' \ge 4)$. Construct a new graph $G'' = G^* - u_1w_1 - u_1w_2 + u_2v + u_2v'$, then we have

$$\begin{aligned} & {}^0R_\alpha(G'') - {}^0R_\alpha(G^*) \\ = \;& 1 + 5^\alpha + (j+1)^\alpha - j^\alpha + (j'+1)^\alpha - j'^\alpha + 2(n-2)^\alpha - 2 \cdot 3^\alpha - 2(n-1)^\alpha \\ > \;& 1 + 5^\alpha - 2 \cdot 3^\alpha + 2(5^\alpha - 4^\alpha) = 1 + 3 \cdot 5^\alpha - 2 \cdot 3^\alpha - 2 \cdot 4^\alpha. \end{aligned}$$

Let $f_4(\alpha) = 1 + 3 \cdot 5^\alpha - 2 \cdot 3^\alpha - 2 \cdot 4^\alpha$. Since

$$f_4'(\alpha) = 3 \ln 5 \cdot 5^\alpha - 2 \ln 4 \cdot 4^\alpha - 2 \ln 3 \cdot 3^\alpha < (3 \ln 5 - 2 \ln 4 - 2 \ln 3) 4^\alpha < 0,$$

we have $f_4(\alpha) > f_4(0) = 0$, i.e., ${}^0R_\alpha(G'') - {}^0R_\alpha(G^*) > 0$, a contradiction.

Subcase 2.3. $n_3 \ge n-4$

Let $u_1, u_2, \ldots, u_{n_3}$ be the vertices of degree 2, then u_i is adjacent to w_1, w_2, w_3 for $1 \le i \le n_3$. Since $n \ge 8$, $n_3 \ge 4$. Construct a new graph $G'' = G^* - u_1w_1 - u_1w_2 + u_2u_3 + u_3u_4$, then we have

$$\begin{aligned} {}^0R_\alpha(G'') - {}^0R_\alpha(G^*) &= 1 + 2 \cdot 4^\alpha + 5^\alpha + 2(n-2)^\alpha - 4 \cdot 3^\alpha - 2(n-1)^\alpha \\ &> 1 + 2 \cdot 4^\alpha + 5^\alpha - 4 \cdot 3^\alpha. \end{aligned}$$

Let $f_5(\alpha) = 1 + 2 \cdot 4^\alpha + 5^\alpha - 4 \cdot 3^\alpha$. Since

$$f_5'(\alpha) = 2 \ln 4 \cdot 4^\alpha + \ln 5 \cdot 5^\alpha - 4 \ln 3 \cdot 3^\alpha < (2 \ln 4 + \ln 5 - 4 \ln 3) 4^\alpha < 0,$$

we have $f_5(\alpha) > f_5(0) = 0$, i.e., ${}^0R_\alpha(G'') - {}^0R_\alpha(G^*) > 0$, a contradiction.

If $n \le 7$ and $n \le m \le (n^2 - 3n + 2)/2$, for any connected (n, m)-graph G with minimum degree $r \ge 2$, it is easy to use some simple Maple programs to list all the possible degree sequences and verify that ${}^0R(L^*) > {}^0R(G)$, since G has at most 7 vertices and 15 edges. Note that at this time, the graph L^* has at least one vertex with degree one. ∎

Note: After this article has been submitted for publication, it came to our attention that similar results are in press in the paper "L. Pavlović, M. Lazić, T. Aleksić, More on 'Connected (n, m)-graphs with minimum and maximum zeroth-order general Randić index', accepted for publication in Discrete Appl. Math." [10]

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