Complete solution to a conjecture on Randić index*

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Abstract

For a graph G, the Randić index $R(G)$ of G is defined by $R(G) = \sum_{u,v} \frac{1}{\sqrt{d(u)d(v)}}$, where $d(u)$ is the degree of a vertex u and the summation runs over all edges uv of G. Let $G(k,n)$ be the set of connected simple graphs of order n with minimum degree k. Bollobás and Erdős once asked for finding the minimum value of the Randić index among the graphs in $G(k,n)$. There have been many partial solutions for this question. In this paper we give a complete solution to the question.

Key words: simple graph; minimum degree; Randić index; minimum value

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1 Introduction

The Randić index $R = R(G)$ of a graph G is defined as follows:

$$R = R(G) = \sum_{u,v} \frac{1}{\sqrt{d(u)d(v)}}, \tag{1.1}$$

where $d(u)$ denotes the degree of a vertex u and the summation runs over all edges uv of G. This topological index was first proposed by Randić [19] in 1975, suitable for measuring the extent of branching of the carbon-atom skeleton of saturated hydrocarbons. Randić himself demonstrated [19] that his index is well correlated with a variety of physico-chemical

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properties of alkanes. The R became one of the most popular molecular descriptors to which three books are devoted [10, 12, 13]. Initially, the Randić index was studied only by chemists [10, 11], but recently it attracted much attention also of mathematicians [13]. One of the mathematical questions asked in connection with R is which graphs in a given class of graphs have maximum and minimum R values [2]. Let $G(k,n)$ be the set of connected simple graphs of order n with minimum degree k. In [6] Fajtlowitcz mentioned that Bollobás and Erdős asked for finding the minimum value of the Randić index among the graphs in $G(k,n)$. The solution of such problem turned out to be difficult, and only a few partial results have been achieved so far. In [2] Bollobás and Erdős found that for a connected graph G

$$R(G) \geq \sqrt{n-1}, \tag{1.2}$$

and the bound is tight if and only if G is a star. The problem for $k = 2$ was solved in [5], which gave a stronger result, say, if the minimum degree is greater or equal to 2, then

$$R(G) \geq \frac{2n-4}{\sqrt{2n-2}} + \frac{1}{n-1}, \tag{1.3}$$

and the bound is tight if and only if $G = K^{\star}_{2,n-2}$ which arises from the complete bipartite graph $K_{2,n-2}$ by joining the vertices in the partite set with 2 vertices by a new edge. In these papers a graph theoretical approach has been used. In other papers [3, 4, 7, 8, 9], a linear programming and a quadratic programming technique [14] for finding extremal graphs has been used.

In [15] the problem was solved for $k = 1$ and $k = 2$, respectively, by using linear programming. Delorme, Favaron and Rautenbach [10] gave a conjecture about this problem. The conjecture in [5] is that the Randić index for graphs in $G(k,n)$, where $1 \leq k \leq n-2$, attains its minimum value for the graph $K^{\star}_{k,n-k}$ which arises from the complete bipartite graph $K_{k,n-k}$ by joining every pair of vertices in the partite set with k vertices by a new edge.

Conjecture 1 ([5]). Let $G = (V,E)$ be a graph of order n with minimum degree k. Then

$$R(G) \geq \frac{k(n-k)}{\sqrt{k(n-1)}} + \binom{k}{2}\frac{1}{n-1} \tag{1.4}$$

where equality holds if and only if $G = K^{\star}_{k,n-k}$.

Using again linear programming, Pavlović [16] proved that Conjecture 1 holds when $k = (n-1)/2$ or $k = n/2$. See also [14] for further results proved by using quadratic programming.

Divnic and Pavlović [17] proved that Conjecture 1 holds when $k \leq n/2$ and $n_k \geq n-k$, where n_k denotes the number of vertices of degree k.

Recently in [1], however, Aouchiche and Hansen showed that Conjecture 1 does not hold in general and proposed a modified conjecture as follows.

Let the graph $\overline{G}_{n,p,k}$ be the complement of a graph $G_{n,p,k}$ composed of a $(n-k-1)$-regular graph on p vertices together with $n-p$ isolated vertices. The minimal counterexample of Conjecture 1 is the graph $\overline{G}_{7,4,5}$, which was given in [1], see Figure 1.

$\overline{G}_{7,4,5}$ $\qquad\qquad$ $G_{7,4,5}$

Figure 1

Let

$$k_n = \begin{cases} \frac{n+2}{2} & \text{if } n \equiv 0 (\text{mod } 4) \\ \frac{n+3}{2} & \text{if } n \equiv 1 (\text{mod } 4) \\ \frac{n+4}{2} & \text{if } n \equiv 2 (\text{mod } 4) \\ \frac{n+3}{2} & \text{if } n \equiv 3 (\text{mod } 4) \end{cases} \qquad p = \begin{cases} \frac{n-2}{2} & \text{if } n \equiv 2 (\text{mod } 4) \text{ and } k \text{ is even} \\ \lceil \frac{n}{2} \rceil & \text{if } n \equiv 3 (\text{mod } 4) \\ \lfloor \frac{n}{2} \rfloor & \text{otherwise} \end{cases} \tag{1.5}$$

For such a graph $G = \overline{G}_{n,p,k}$,

$$R(G) = \frac{(n-p)(n-p-1)}{2(n-1)} + \frac{p(p+k-n)}{2k} + \frac{p(n-p)}{\sqrt{k(n-1)}}$$

Using these results, the authors of [1] gave the following Conjecture 2 as a modification of Conjecture 1.

Conjecture 2 ([1]). Let $G = (V, E)$ be a graph of order n with minimum degree k, and k_n and p be given in (1.5). Then

$$R(G) \geq \begin{cases} \frac{k(k-1)}{2(n-1)} + \frac{k(n-k)}{\sqrt{k(n-1)}} & \text{if } k < k_n \\ \frac{(n-p)(n-p-1)}{2(n-1)} + \frac{p(p+k-n)}{2k} + \frac{p(n-p)}{\sqrt{k(n-1)}} & \text{if } k_n \leq k \leq n-2, \end{cases}$$

where equality holds if and only if G is $K^{\star}_{k,n-k}$ for $k < k_n$, and $\overline{G}_{n,p,k}$ for $k \geq k_n$.

In this paper, we want to completely solve the Bollobás and Erdős' question of finding the minimum value of the Randić index for the graphs in $G(k,n)$. As usual, we formulate the question into a mathematical programming problem. Denote by n_i the number of vertices of degree i in G, and by $x_{i,j}$ ($x_{i,j} \geq 0$) the number of edges joining the vertices of degrees i and j in G. The mathematical description of our problem is as follows:

$$min\ R(G) = \sum_{\substack{k \leq i \leq n-1 \\ i \leq j \leq n-1}} \frac{x_{i,j}}{\sqrt{ij}}$$

subject to:

$$\sum_{\substack{j=k \\ j \neq i}}^{n-1} x_{i,j} + 2x_{i,i} = in_i \quad \text{for} \quad k \leq i \leq n-1; \tag{1.6}$$

$$n_k + n_{k+1} + \cdots + n_{n-1} = n; \tag{1.7}$$

$$x_{i,j} \leq n_i n_j \quad \text{for} \quad k \leq i \leq n-1 \quad i < j \leq n-1; \tag{1.8}$$

$$x_{i,i} \leq \binom{n_i}{2} \quad \text{for} \quad k \leq i \leq n-1; \tag{1.9}$$

$$x_{i,j},\ n_i \text{ are nonnegative integers, for } k \leq i \leq j \leq n-1. \tag{1.10}$$

Obviously, (1.6)-(1.10) define a nonlinearly constrained optimization problem.

2 Main result

Denote

$$p = \begin{cases} \frac{n}{2} & \text{if } n \equiv 0 (\text{mod } 4) \\ \lfloor \frac{n}{2} \rfloor \text{ or } \lceil \frac{n}{2} \rceil & \text{if } n \equiv 1 (\text{mod } 4) \text{and } k \text{ is even} \\ \lfloor \frac{n}{2} \rfloor & \text{if } n \equiv 1 (\text{mod } 4) \text{and } k \text{ is odd} \\ \frac{n-2}{2} \text{ or } \frac{n+2}{2} & \text{if } n \equiv 2 (\text{mod } 4) \text{and } k \text{ is even} \\ \frac{n}{2} & \text{if } n \equiv 2 (\text{mod } 4) \text{and } k \text{ is odd} \\ \lfloor \frac{n}{2} \rfloor \text{ or } \lceil \frac{n}{2} \rceil & \text{if } n \equiv 3 (\text{mod } 4) \text{and } k \text{ is even} \\ \lceil \frac{n}{2} \rceil & \text{if } n \equiv 3 (\text{mod } 4) \text{and } k \text{ is odd.} \end{cases} \tag{2.11}$$

Theorem 2.1 *Let $G = (V, E)$ be a graph of order n with minimum degree k, and p be given in* (2.11)*. Then we have*

$$R(G) \geq \begin{cases} \frac{k(k-1)}{2(n-1)} + \frac{k(n-k)}{\sqrt{k(n-1)}} & \text{if } k \leq n/2 \\ \frac{(n-p)(n-p-1)}{2(n-1)} + \frac{p(p+k-n)}{2k} + \frac{p(n-p)}{\sqrt{k(n-1)}} & \text{if } k > n/2 \end{cases}$$

where equality holds if and only if G is $K^{\star}_{k,n-k}$ for $k \le n/2$, and $\overline{G}_{n,p,k}$ for $k > n/2$.

Proof. It is easy to see that $n_{n-1} \le k$, or the minimum degree of a graph in $G(k,n)$ would be larger than k. Therefore we only need to consider the case when $n_{n-1} \le k$. Let $n_{n-1} = k - t$ for some integer t such that $0 \le t \le k$, and let R_{k-t} denote the Randić index for any graph in $G(k,n)$ with $n_{n-1} = k - t$ $(0 \le t \le k)$. Since $x_{i,n-1} = n_i n_{n-1}$ for $k \le i \le n-2$ and $x_{n-1,n-1} = n_{n-1}(n_{n-1}-1)/2$, we have

$$\begin{aligned}
R_{k-t} &= \sum_{\substack{k\le i\le n-1\\ i\le j\le n-1}} \frac{x_{i,j}}{\sqrt{ij}} = \sum_{i=k}^{n-2} \frac{n_i n_{n-1}}{\sqrt{i(n-1)}} + \frac{n_{n-1}(n_{n-1}-1)}{2(n-1)} \\
&\quad + \frac{1}{2}\sum_{j=k}^{n-2}\Big(\frac{x_{k,j}}{\sqrt{kj}} + \cdots + \frac{x_{j-1,j}}{\sqrt{(j-1)j}} + 2\frac{x_{j,j}}{\sqrt{jj}} + \frac{x_{j+1,j}}{\sqrt{j(j+1)}} + \cdots + \frac{x_{j,n-2}}{\sqrt{j(n-2)}}\Big) \\
&\ge \sum_{i=k}^{n-2} \frac{n_i n_{n-1}}{\sqrt{i(n-1)}} + \frac{n_{n-1}(n_{n-1}-1)}{2(n-1)} + \frac{1}{2}\Big(\frac{2x_{k,k}}{\sqrt{kk}} + \frac{x_{k,k+1}}{\sqrt{k(k+1)}} + \cdots + \frac{x_{k,n-2}}{\sqrt{k(n-2)}}\Big) \\
&\quad + \frac{1}{2}\sum_{j=k+1}^{n-2} \frac{x_{k,j} + \cdots + x_{j-1,j} + 2x_{j,j} + x_{j,j+1} + \cdots + x_{j,n-2}}{\sqrt{j(n-1)}} \qquad (2.12) \\
&= \sum_{i=k}^{n-2} \frac{n_i n_{n-1}}{\sqrt{i(n-1)}} + \frac{n_{n-1}(n_{n-1}-1)}{2(n-1)} + \frac{1}{2}\Big(\frac{2x_{k,k}}{\sqrt{kk}} + \frac{x_{k,k+1}}{\sqrt{k(k+1)}} + \cdots + \frac{x_{k,n-2}}{\sqrt{k(n-2)}}\Big) \\
&\quad + \frac{1}{2}\sum_{j=k+1}^{n-2} \frac{jn_j - n_j n_{n-1}}{\sqrt{j(n-1)}} \qquad (2.13) \\
&= \frac{1}{2\sqrt{n-1}}\sum_{j=k+1}^{n-2}\sqrt{j}n_j + \frac{n_{n-1}}{2\sqrt{n-1}}\sum_{j=k+1}^{n-2}\frac{n_j}{\sqrt{j}} + \frac{n_{n-1}(n_{n-1}-1)}{2(n-1)} \\
&\quad + \frac{1}{2}\Big(\frac{2x_{k,k}}{\sqrt{kk}} + \frac{x_{k,k+1}}{\sqrt{k(k+1)}} + \cdots + \frac{x_{k,n-2}}{\sqrt{k(n-2)}}\Big) + \frac{n_k n_{n-1}}{\sqrt{k(n-1)}},
\end{aligned}$$

where inequality (2.12) holds because $\frac{1}{\sqrt{i}} \ge \frac{1}{\sqrt{n-1}}$ for $k+1 \le i \le n-2$, and equality (2.13) holds because of (1.6). After substitution of $n_{n-1} = k - t$ and $n_k = n - k + t - n_{k+1} - n_{k+2} - \cdots - n_{n-2}$ into the last equality, we have

$$\begin{aligned}
R_{k-t} &\ge \frac{(k-t)(k-t-1)}{2(n-1)} + \frac{(k-t)(n-k+t)}{\sqrt{k(n-1)}} \\
&\quad + \sum_{j=k+1}^{n-2}\left(\sqrt{j} - \sqrt{k} - (k-t)\Big(\frac{1}{\sqrt{k}} - \frac{1}{\sqrt{j}}\Big) + \frac{t}{\sqrt{k}}\right)\frac{n_j}{2\sqrt{n-1}} \\
&\quad + \frac{1}{2}\Big(\frac{2x_{k,k}}{\sqrt{kk}} + \frac{x_{k,k+1}}{\sqrt{k(k+1)}} + \cdots + \frac{x_{k,n-2}}{\sqrt{k(n-2)}}\Big).
\end{aligned}$$

Since $\sqrt{kj} > k - t$ for $k+1 \le j \le n-2$, we have $\sqrt{j} - \sqrt{k} > (k-t)\frac{\sqrt{j}-\sqrt{k}}{\sqrt{kj}}$, i.e., $\sqrt{j} - \sqrt{k} > (k-t)(\frac{1}{\sqrt{k}} - \frac{1}{\sqrt{j}})$. Thus $\sqrt{j} - \sqrt{k} - (k-t)(\frac{1}{\sqrt{k}} - \frac{1}{\sqrt{j}}) + \frac{t}{\sqrt{k}} > 0$. Since if $n_j = 0$ then $x_{i,j} = 0$

for $k \le i \le j \le n-2$, we then have

$$\frac{(k-t)(k-t-1)}{2(n-1)} + \frac{(k-t)(n-k+t)}{\sqrt{k(n-1)}} + \sum_{j=k+1}^{n-2}\left(\sqrt{j}-\sqrt{k}-(k-t)(\frac{1}{\sqrt{k}}-\frac{1}{\sqrt{j}})+\frac{t}{\sqrt{k}}\right)\frac{n_j}{2\sqrt{n-1}}$$
$$+\frac{1}{2}(\frac{2x_{k,k}}{\sqrt{kk}}+\frac{x_{k,k+1}}{\sqrt{k(k+1)}}+\cdots+\frac{x_{k,n-2}}{\sqrt{k(n-2)}})$$
$$\ge \frac{(k-t)(k-t-1)}{2(n-1)} + \frac{(k-t)(n-k+t)}{\sqrt{k(n-1)}} + \frac{x_{k,k}}{k}.$$

Notice that equalities hold in all the above inequalities if and only if $n_j = 0,\ j = k+1, k+2, \cdots, n-2$. Thus,

$$R_{k-t} \ge \frac{(k-t)(k-t-1)}{2(n-1)} + \frac{(k-t)(n-k+t)}{\sqrt{k(n-1)}} + \frac{x_{k,k}}{k},$$

where equality holds if and only if $n_j = 0,\ j = k+1, k+2, \cdots, n-2$.

We know that if $n_j = 0,\ j = k+1, k+2, \cdots, n-2$, then $n_k = n-k+t,\ n_{n-1} = k-t$, $x_{k,k} = (n-k+t)t/2,\ x_{n-1,n-1} = (k-t)(k-t-1)/2$ and all other $x_{i,j}$ and $x_{i,i}$ are equal to zero. Therefore,

$$R_{k-t} \ge \frac{(k-t)(k-t-1)}{2(n-1)} + \frac{(k-t)(n-k+t)}{\sqrt{k(n-1)}} + \frac{(n-k+t)t}{2k},$$

where equality holds if and only if $n_j = 0,\ j = k+1, k+2, \cdots, n-2$.

Let

$$f(k,t) = \frac{(k-t)(n-k+t)}{\sqrt{k(n-1)}} + \frac{(k-t)(k-t-1)}{2(n-1)} + \frac{(n-k+t)t}{2k}.$$

We only need to get the minimum value of $f(k,t)$, by distinguishing two cases.

Case 1. $k \le n/2$.

Since $\partial f(k,t)/\partial t = \frac{n+2t-2k}{2}(\frac{1}{\sqrt{k}}-\frac{1}{\sqrt{n-1}})^2 \ge 0$, and $\partial f(k,t)/\partial t > 0$ strictly holds except for $k-t = n/2$, i.e., $k = n/2+t$, we know that $f(k,t)$ attains its minimum if and only if $t = 0$ since $k \le n/2$ in this case.

So, in this case we can conclude that the Randić index attains its minimum in $G(k,n)$ if and only if all the above equalities hold, which means that $n_k = n-k,\ n_{n-1} = k,\ n_j = 0,\ j = k+1, \cdots, n-2,\ x_{n-1,n-1} = \binom{k}{2}$ and all other $x_{i,j}, x_{i,i}$ are equal to zero. Therefore, a graph G in $G(k,n)$ attains the minimum value of the Randić index if and only if $G = K^*_{k,n-k}$ for $k \le n/2$.

Case 2. $n-2 \geq k > n/2$.

Let $\partial f(k,t)/\partial t = \frac{n+2t-2k}{2}(\frac{1}{\sqrt{k}} - \frac{1}{\sqrt{n-1}})^2 = 0$. Then $t = k - n/2$. Since $\partial^2 f(k,t)/\partial t^2 = (\frac{1}{\sqrt{k}} - \frac{1}{\sqrt{n-1}})^2 > 0$, $f(k,t)$ attain its minimum if and only if $t = k - n/2$. Then we have $n_k = n/2$, $x_{k,k} = n(2k-n)/2$ and $x_{n-1,n-1} = n(n-2)/8$. Next, we need to check whether they are integers or not, since the obtained solutions have no graph theoretical meaning when one of the three values, namely, $x_{k,k} = (n-k+t)t/2$, $x_{n-1,n-1} = (k-t)(k-t-1)/2$ and t, is not an integer.

Subcase 2.1. $n \equiv 0 \pmod 4$.

We can easily check that $t = k - n/2$, $x_{k,k} = n/2$ and $x_{n-1,n-1} = n(n-2)/8$ are integers in this case. Therefore, a graph G in $G(k,n)$ attains the minimum value of the Randić index if and only if $G = \overline{G}_{n,n/2,k}$ in the case $n \equiv 0 \pmod 4$.

Subcase 2.2. $n \equiv 1 \pmod 4$.

We see first that $t = k - n/2$ is not an integer in this case. Therefore, the obtained solutions have no graph theoretical meaning. Then t can not attain $k - n/2$ if we want to get the minimum value of the Randić index in $G(k,n)$. We then let $t \leq k - \frac{n+1}{2}$ or $t \geq k - \frac{n-1}{2}$.

For $t \leq k - \frac{n+1}{2}$, we have $n + 2t - 2k \leq -1 < 0$. Thus $\partial f(k,t)/\partial t < 0$. Therefore, $f(k,t)$ attains its minimum if and only if $t = k - \frac{n+1}{2}$ in this case. And then $n_k = (n-1)/2$, $n_{n-1} = (n+1)/2$, $x_{k,k} = (n-1)(2k-n-1)/8$, $x_{n-1,n-1} = (n+1)(n-1)/2$ all are integers. So, $min\ f(k,t) = \frac{(n-1)(2k-n-1)}{8k} + \frac{(n+1)(n-1)}{4\sqrt{k(n-1)}} + \frac{(n+1)(n-1)}{8(n-1)}$.

For $t \geq k - \frac{n-1}{2}$, we have $n + 2t - 2k \geq 1 > 0$. Thus $\partial f(k,t)/\partial t > 0$. Therefore, $f(k,t)$ attains its minimum if and only if $t = k - \frac{n-1}{2}$ in this case. And then $n_k = (n+1)/2$, $n^*_{n-1} = (n-1)/2$, $x_{k,k} = (n+1)(2k-n+1)/8$, $x^*_{n-1,n-1} = (n-1)(n-3)/2$ all are integers if k is even. So, $min\ f(k,t) = \frac{(n+1)(2k-n+1)}{8k} + \frac{(n+1)(n-1)}{4\sqrt{k(n-1)}} + \frac{(n-1)(n-3)}{8(n-1)} = \frac{(n-1)(2k-n-1)}{8k} + \frac{(n+1)(n-1)}{4\sqrt{k(n-1)}} + \frac{(n+1)(n-1)}{8(n-1)}$, which is the same as the minimum value for the above case when $t \leq k - \frac{n+1}{2}$.

Therefore, a graph G in $G(k,n)$ attains the minimum value of the Randić index if and only if G is $\overline{G}_{n,\lfloor \frac{n}{2} \rfloor,k}$ for k both even and odd, or $\overline{G}_{n,\lceil \frac{n}{2} \rceil,k}$ for k even in the case $n \equiv 1 \pmod 4$.

Subcase 2.3. $n \equiv 2 \pmod 4$.

We can easily check that $t = k - n/2$, $x_{k,k} = n(2k - n)/8$ and $x_{n-1,n-1} = n(n - 2)/8$ are integers if k is odd in this case. Therefore, a graph G in $G(k, n)$ attains the minimum value of the Randić index if and only if G is $\overline{G}_{n,n/2,k}$ for k odd in the case $n \equiv 1 \pmod 4$.

If k is even, then $x_{k,k} = n(2k - n)/8$ is not an integer in this case, which means that t can not attain $k - n/2$ if we want to get the minimum value of the Randić index in $G(k, n)$. We then let $t \leq k - \frac{n+2}{2}$ or $t \geq k - \frac{n-2}{2}$.

For $t \leq k - \frac{n+2}{2}$, we have $n + 2t - 2k \leq -2 < 0$. Thus $\partial f(k, t)/\partial t < 0$. Therefore, $f(k, t)$ attains its minimum if and only if $t = k - \frac{n+2}{2}$ in this case. And then $n_k = (n-2)/2$, $n_{n-1} = (n + 2)/2$, $x_{k,k} = (n - 2)(2k - n - 2)/8$, $x_{n-1,n-1} = n(n + 2)/2$ all are integers. So, $min\ f(k, t) = \frac{(n-2)(2k-n-2)}{8k} + \frac{(n-2)(n+2)}{4\sqrt{k(n-1)}} + \frac{n(n+2)}{8(n-1)}$.

For $t \geq k - \frac{n-2}{2}$, we have $n + 2t - 2k \geq 2 > 0$. Thus $\partial f(k, t)/\partial t > 0$. Therefore, $f(k, t)$ attains its minimum if and only if $t = k - \frac{n-2}{2}$ in this case. And then $n_k = (n+2)/2$, $n^*_{n-1} = (n - 2)/2$, $x_{k,k} = (n + 2)(2k - n + 2)/8$, $x_{n-1,n-1} = (n - 2)(n - 4)/2$ all are integers. So, $min\ f(k, t) = \frac{(n+2)(2k-n+2)}{8k} + \frac{(n-2)(n+2)}{4\sqrt{k(n-1)}} + \frac{(n-2)(n-4)}{8(n-1)} = \frac{(n-2)(2k-n-2)}{8k} + \frac{(n-2)(n+2)}{4\sqrt{k(n-1)}} + \frac{n(n+2)}{8(n-1)}$, which is the same as the minimum value for the above case when $t \leq k - \frac{n+2}{2}$.

Therefore, in the case $n \equiv 2 \pmod 4$ and k is odd, a graph G in $G(k, n)$ attains the minimum value of the Randić index if and only if $G = \overline{G}_{n,\frac{n}{2},k}$.

In the case $n \equiv 2 \pmod 4$ and k is even, a graph G in $G(k, n)$ attains the minimum value of the Randić index if and only if $G = \overline{G}_{n,\frac{n-2}{2},k}$ or $\overline{G}_{n,\frac{n+2}{2},k}$.

Subcase 2.4. $n \equiv 3 \pmod 4$.

Similar to the proof of Subcase 2.2, we can get that a graph G in $G(k, n)$ attains the minimum value of the Randić index if and only if G is $\overline{G}_{n,\lceil\frac{n}{2}\rceil,k}$ for k both even and odd, or $\overline{G}_{n,\lfloor\frac{n}{2}\rfloor,k}$ for k even.

The proof is now complete. ∎

References

[1] M. Aouchiche, P. Hansen, On a conjecture about the Randić index, Discrete Math. 307(2)(2007), 262-265.

[2] B. Bollobás, P. Erdős, Graphs of extremal weights, Ars Combin. 50(1998), 225-233.

[3] G. Caporossi, I. Gutman, P. Hansen, Variable neighborhood search for extremal graphs IV: Chemical trees with extremal connectivity index, Computers and Chemistry 23(1999), 469-477.

[4] G. Caporossi, I. Gutman, P. Hansen, Lj. Pavlović, Graph with maximum connectively index, Computational Biology & Chemistry 27(2003), 85-90.

[5] C. Delorme, O. Favaron, D. Rautenbach, On the Randić index, Discrete Math. 257(1)(2002), 29-38.

[6] S. Fajtlowicz, Written on the wall: Conjectures derived on the basis of the program Galatea Gabriella Graffiti, University of Houston, 1998.

[7] M. Fischermann, A. Hoffmann, D. Rautenbach, L. Volkmann, A linear-programming approach to the generalized Randić index, Discrete Appl. Math. 128(2003), 375-385.

[8] I. Gutman, O. Miljkovic, G. Caporossi, P. Hansen, Alkanes with small and large Randić connectivity indices, Chem. Phys. Lett. 306(1999), 366-372.

[9] I. Gutman, Lj. Pavlović, O. Miljkovic, On graphs with extremal connectivity indices, Bulletin de l'Academie Serbe des Sciences er des Arts 25(2000), 1-14.

[10] L.B. Kier, L.H. Hall, Molecular Connectivity in Chemistry and Drug Research, Academic Press, New York, 1976.

[11] 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.

[12] L.B. Kier, L.H. Hall, Molecular Connectivity in structure-Activity Analysis, Research Studies Press-Wiley, Chichester(UK), 1986.

[13] X. Li, I. Gutman, Mathematical Aspects of Randic-Type Molecular Structure Descriptors, Mathematical Chemistry Monographs No.1, Kragujevac, 2006, pp.VI+330.

[14] N. Limic, H. Psasgic, C. Rnjak, Linearno i nelinearno programiranje, Informator, Zagreb(HR), 1978.

[15] Lj. Pavlović, Graphs with extremal Randić index when the minimum degree of vertices is two, Kragujevac J. Math. 25(2003), 55-63.

[16] Lj. Pavlović, On the conjecture of Delorme, Favaron and Rautenbach about the Randić index, European J. Operational Research 180(2007), 369-377.

[17] Lj. Pavlović, T. Divnic, A quadratic programming approach to the Randić index. European J. Operational Research 176(2007), 435-444.

[18] Lj. Pavlović, I. Gutman, Graph with extremal connectivity index, Novi Sad J. Math. 31(2)(2001), 53-58.

[19] M. Randić, On characterization of molecular branching, J. Amer. Chem. Soc. 97(1975), 6609-6615.