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GRAPHS WITH EXTREMAL RANDIĆ INDEX WHEN THE MINIMUM DEGREE OF VERTICES IS TWO

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Abstract. Let $G(2,n)$ be a connected graph without multiple edges which has n vertices and the minimum degree of vertices is 2. The Randić index is: $\chi = \sum_{(uv)}(\delta_u\delta_v)^{-1/2}$, where δ_u is the degree of vertex u and the summation goes over all edges (uv) of G. In this paper we offer another technique based on linear programming to find graphs on which the Randić index attains minimum value. The extremal graphs have $n-2$ vertices of degree 2 and 2 vertices of degree $n-1$.

1. INTRODUCTION

Let $G(k,n)$ be a connected graph without multiple edges which has n vertices and the minimum degree of vertices is k. Denote by u its vertex and by δ_u the degree of the vertex u, that is the number of edges of which u is an endpoint. Denote further by (uv) the edge whose endpoints are the vertices u and v and by n_i the number of vertices of degree i. In 1975 Randić proposed a topological index, suitable for measuring the extent of branching of the carbon-atom skeleton of saturated hydrocarbons. The Randić index defined in [10] is: $\chi = \sum_{(uv)}(\delta_u\delta_v)^{-1/2}$, where the summation goes over all edges of G. Randić himself demonstrated [10] that his index is well correlated with a variety of physico-chemical properties of alkanes. χ became one of the most popular molecular descriptors to which two books are devoted ([7], [8]).

One of the mathematical questions asked in connection with χ is which graphs with given class of graphs have maximum and minimum χ values ([1], [2], [4], [5]). In [3] Fajtlowitcz mentions that Bollobás and Erdős asked for the minimum value on the Randić index for the graphs $G(k, n)$. The solution of such problems turned out to be difficult, and only a few partial results have been achieved so far. In [1] Bollobás and Erdős found the extremal graph when $k = 1$. It is the star. For $k = 2$ the problem is solved in [6] and the extremal graph is a "double star", that is, it has to have $n_2 = n-2$ and $n_{n-1} = 2$. In [1] and [6] is used a technic proposed by Bollobás and Erdős. In [9] the problem is solved for $k = 1$ using linear programming. In this paper we use linear programming to solve problem for $k = 2$. This technique is more systematic and more promising for general case ($k \geq 3$).

2. MATHEMATICAL DESCRIPTION OF THE PROBLEM

At first, we will give some linear equalities which describe better this problem. Denote by $x_{i,j}$, ($x_{i,j} \geq 0$), the number of edges joining the vertices of degrees i and j. Mathematically description of the problem (P) is:

$$\min \sum_{\substack{2\leq i\leq n-1\\ i\leq j\leq n-1}} \frac{x_{i,j}}{\sqrt{ij}}$$

under constraints:

$$\begin{array}{rrrcrl} 2x_{2,2}+ & x_{2,3}+ & x_{2,4}+ & \ldots & + \quad x_{2,n-1} & = 2n_2 \\ x_{2,3}+ & 2x_{3,3}+ & x_{3,4}+ & \ldots & + \quad x_{3,n-1} & = 3n_3 \\ x_{2,4}+ & x_{3,4}+ & 2x_{4,4}+ & \ldots & + \quad x_{4,n-1} & = 4n_4 \\ & & & \vdots & & \\ x_{2,n-1}+ & x_{3,n-1}+ & x_{4,n-1}+ & \ldots & +2x_{n-1,n-1} & = (n-1)n_{n-1} \end{array} \qquad (A)$$

and

$$n_2 + n_3 + n_4 + \ldots + n_{n-1} = n \qquad (B)$$

These constraints do not completely determine the problem. If we try to solve this problem of linear programming, we will obtain solutions which are not graphical (except for $k = 1$).To describe better this problem we have to add the next constraints: $x_{i,j} \leq n_i n_j$ for $2 \leq i \leq n-1$, $i < j \leq n-1$ and $x_{i,i} \leq \binom{n_i}{2}$ for $2 \leq i \leq n-1$, which much more complicate the problem. It is now the problem of quadratic programming. To avoid the complicacy of these quadratic inequalities we will give to n_{n-1} all possible values and solve the upper problem using linear programming.

3. RESULTS

Theorem 1. Let $G(2, n)$ be a connected graph without multiple edges which has n vertices and the minimum degree of vertices is 2. The minimum value of the Randić index is:

$$\chi^* = \frac{2(n-2)}{\sqrt{2(n-1)}} + \frac{1}{n-1}$$

This value is attained on the graph with $n_2 = n-2$, $n_{n-1} = 2$, $n_3 = n_4 = \ldots = n_{n-2} = 0$, $x_{2,n-1} = 2(n-2)$, $x_{n-1,n-1} = 1$ and all other $x_{i,j}$ and $x_{i,i}$ being equal to 0.

Proof. Since $n_{n-1} \leq 2$, when the minimum degree of vertices is 2, we will consider three cases: $n_{n-1} = 2$, $n_{n-1} = 1$ and $n_{n-1} = 0$. Denote by χ_i the value of the Randić index when $n_{n-1} = i$, $i = 0, 1, 2$. We will use the next equalities: $x_{i,n-1} = n_i n_{n-1}$ for $i = 2, 3, \ldots, n-2$ and $x_{n-1,n-1} = \binom{n_{n-1}}{2}$.

Case 1: $n_{n-1} = 2$. Since $x_{i,n-1} = 2n_i$ for $i = 2, 3, \ldots, n-2$ and $x_{n-1,n-1} = 1$, constraints (A) become: $x_{2,j} + \ldots + x_{j-1,j} + 2x_{j,j} + x_{j+1,j} + \ldots x_{j,n-2} = jn_j - 2n_j$ for $j = 2, 3, \ldots, n-2$. We have:

$$\chi_2 = \sum_{\substack{2 \leq i \leq n-1 \\ i \leq j \leq n-1}} \frac{x_{i,j}}{\sqrt{ij}} = \sum_{j=2}^{n-2} \frac{2n_j}{\sqrt{j(n-1)}} + \frac{1}{n-1} +$$

$$\frac{1}{2}\sum_{j=2}^{n-2}(\frac{x_{2,j}}{\sqrt{2j}}+\ldots+\frac{x_{j-1,j}}{\sqrt{(j-1)j}}+2\frac{x_{j,j}}{\sqrt{jj}}+\frac{x_{j,j+1}}{\sqrt{(j(j+1)}}+\ldots+\frac{x_{j,n-2}}{\sqrt{(j(n-2)}})\geq$$
$$\sum_{j=2}^{n-2}\frac{2n_j}{\sqrt{j(n-1)}}+\frac{1}{n-1}+$$
$$\frac{1}{2}\sum_{j=2}^{n-2}\frac{x_{2,j}+\ldots+x_{j-1,j}+2x_{j,j}+x_{j+1,j}+\ldots x_{j,n-2}}{\sqrt{j(n-1)}}=$$
$$\sum_{j=2}^{n-2}\frac{2n_j}{\sqrt{j(n-1)}}+\frac{1}{n-1}+\frac{1}{2}\sum_{j=2}^{n-2}\frac{jn_j-2n_j}{\sqrt{j(n-1)}}=$$
$$\frac{1}{2\sqrt{n-1}}\sum_{j=2}^{n-2}\sqrt{j}n_j+\frac{1}{\sqrt{n-1}}\sum_{j=2}^{n-2}\frac{n_j}{\sqrt{j}}+\frac{1}{n-1}$$

because $\frac{1}{\sqrt{i}}\geq\frac{1}{\sqrt{n-1}}$ for $2\leq i\leq n-2$. After substitution of $n_2=n-2-n_3-n_4-\ldots-n_{n-2}$ in the last equality, we have:

$$\chi_2=\frac{2(n-2)}{\sqrt{2(n-1)}}+\frac{1}{n-1}+\sum_{j=3}^{n-2}(\sqrt{j}-\sqrt{2}+2(\frac{1}{\sqrt{j}}-\frac{1}{\sqrt{2}}))\frac{n_j}{2\sqrt{n-1}}$$

Since $\sqrt{j}-\sqrt{2}+2(\frac{1}{\sqrt{j}}-\frac{1}{\sqrt{2}})\geq 0$ for $3\leq j\leq n-2$, this function attains minimum for $n_j=0,\ \ j=3,4,\ldots,n-2$. When $n_{n-1}=2$ the minimum value of the Randić index is:

$$\chi_2^*=\frac{2(n-2)}{\sqrt{2(n-1)}}+\frac{1}{n-1}$$

The extremal graph must have $n_2=n-2$, $n_3=n_4=\ldots=n_{n-2}=0$, $n_{n-1}=2$, $x_{2,n-1}=2(n-2)$, $x_{n-1,n-1}=1$ and all other $x_{i,j}$ and $x_{i,i}$ are equal to 0.

Case 2: $n_{n-1}=1$. After substitution of $x_{i,n-1}=n_i$ for $i=2,3,\ldots,n-2$ and $x_{n-1,n-1}=0$ in the constraints (A), they become (A'):

$$\begin{array}{rrrcrl}
2x_{2,2}+ & x_{2,3}+ & x_{2,4}+ & \ldots & + \quad x_{2,n-2} & = n_2\\
x_{2,3}+ & 2x_{3,3}+ & x_{3,4}+ & \ldots & + \quad x_{3,n-2} & = 2n_3\\
x_{2,4}+ & x_{3,4}+ & 2x_{4,4}+ & \ldots & + \quad x_{4,n-2} & = 3n_4\\
 & & & \vdots & & \\
x_{2,n-2}+ & x_{3,n-2}+ & x_{4,n-2}+ & \ldots & +2x_{n-2,n-2} & = (n-3)n_{n-2}
\end{array} \qquad (A')$$

Since $n_{n-1} = 1$, equality (B) becomes (B'):

$$n_2 + n_3 + n_4 + \ldots + n_{n-2} = n - 1 \tag{B'}$$

We have the next problem of linear programming: $\min \chi_1$ under constraints (A') and (B'). The basic variables are n_i for $i = 2, 3, \ldots, n-1$, $x_{2,n-2}$, $x_{i,n-1} = n_i$ for $i = 2, 3, \ldots, n-2$ and $x_{n-1,n-1} = 0$. It is easy to find n_i for $i = 3, 4, \ldots, n-3$ from constraints (A'):

$$n_i = \frac{x_{2,i} + \ldots + x_{i-1,i} + 2x_{i,i} + x_{i,i+1} + \ldots + x_{i,n-2}}{i-1} \tag{1}$$

Using the first and the last constraint of (A') and constraint (B') we find:

$$n_2 = \frac{(n-1)(n-3)}{n-2} + \frac{2x_{2,2}}{n-2} - \sum_{j=3}^{n-3} \frac{(n-j-2)x_{2,j}}{(j-1)(n-2)} - \sum_{\substack{3 \le i \le n-2 \\ i \le j \le n-2}} \left(\frac{n-3}{i-1} + \frac{n-3}{j-1}\right)\frac{x_{i,j}}{n-2}, \tag{2}$$

$$n_{n-2} = \frac{n-1}{n-2} - \sum_{\substack{2 \le i \le n-3 \\ i \le j \le n-3}} \left(\frac{1}{i-1} + \frac{1}{j-1}\right)\frac{x_{i,j}}{n-2} - \sum_{i=3}^{n-3} \left(\frac{1}{i-1} - 1\right)\frac{x_{i,n-2}}{n-2} + \frac{2x_{n-2,n-2}}{n-2}, \tag{3}$$

$$x_{2,n-2} = \frac{(n-1)(n-3)}{(n-2)} - \sum_{j=2}^{n-3} \left(1 + \frac{n-j-2}{(j-1)(n-2)}\right)x_{2,j} - \sum_{\substack{3 \le i \le n-2 \\ i \le j \le n-2}} \left(\frac{n-3}{i-1} + \frac{n-3}{j-1}\right)\frac{x_{i,j}}{n-2} \tag{4}$$

After substitution of $x_{2,n-2}$ from (4), $x_{i,n-1} = n_i$, $i = 2, 3, \ldots, n-2$ from (1), (2) and (3) into χ_1, we have:

$$\begin{aligned}\chi_1 &= \left(\frac{n-3}{\sqrt{2(n-2)}} + \frac{n-3}{\sqrt{2(n-1)}} + \frac{1}{\sqrt{(n-2)(n-1)}}\right)\frac{n-1}{n-2} + \\ &\quad \sum_{j=2}^{n-3} a_{2,j}x_{2,j} + \sum_{\substack{3 \le i \le n-2 \\ i \le j \le n-2}} a_{i,j}x_{i,j}\end{aligned}$$

where

$$\begin{aligned}a_{i,j} &= \frac{1}{\sqrt{ij}} - \frac{\frac{1}{n-2}\left(\frac{n-3}{i-1} + \frac{n-3}{j-1}\right)}{\sqrt{2(n-2)}} - \frac{\frac{1}{n-2}\left(\frac{n-3}{i-1} + \frac{n-3}{j-1}\right)}{\sqrt{2(n-1)}} + \frac{\frac{1}{i-1}}{\sqrt{i(n-1)}} + \frac{\frac{1}{j-1}}{\sqrt{j(n-1)}} - \\ &\quad \frac{\frac{1}{n-2}\left(\frac{1}{i-1} + \frac{1}{j-1}\right)}{\sqrt{(n-2)(n-1)}}\end{aligned}$$

We will prove that all functions $a_{i,j}$ are nonnegative for corresponding i and j.

Since

$$\frac{\partial^2}{\partial j^2}((n-2)(i-1)(j-1)a_{i,j}) = \frac{(n-2)(i-1)}{4\sqrt{j^5}}(\frac{3}{\sqrt{n-1}} - \frac{j+3}{\sqrt{i}}) \leq$$

$$\frac{(n-2)(i-1)}{4\sqrt{j^5}}(\frac{3}{\sqrt{n-1}} - \frac{i+3}{\sqrt{i}}) \leq \frac{(n-2)(i-1)}{4\sqrt{j^5}}(\frac{3}{\sqrt{n-1}} - \frac{5}{\sqrt{2}}) \leq 0$$

for $n \geq 2$, because $j \geq i \geq 2$, the function $(n-2)(i-1)(j-1)a_{i,j}$ is concave on j. We have to check that $a_{i,i}$ and $a_{i,n-2}$ are nonnegative in order to conclude that $a_{i,j} \geq 0$ for $i \leq j \leq n-2$ and $2 \leq i \leq n-2$. We begin with $a_{i,i}$. Since

$$\frac{\partial}{\partial i}((n-2)(i-1)a_{i,i}) = \frac{n-2}{\sqrt{i^3}}(\frac{1}{\sqrt{i}} - \frac{1}{\sqrt{n-1}}) \geq 0$$

because $i \leq n-1$, it holds $(n-2)(i-1)a_{i,i} \geq (n-2)a_{2,2}$. For $n \geq 6$, holds:

$$(n-2)a_{2,2} = \frac{n-2}{2} - \frac{2(n-3)}{\sqrt{2(n-2)}} + \frac{2}{\sqrt{n-1}}(\frac{1}{\sqrt{2}} - \frac{1}{\sqrt{n-2}}) \geq 0 \tag{5}$$

because $\frac{n-2}{2} \geq \frac{2(n-3)}{\sqrt{2(n-2)}}$ for $n \geq 10$ and $\frac{1}{\sqrt{2}} \geq \frac{1}{\sqrt{n-2}}$ for $n \geq 4$. We can see by numerical checking that $a_{2,2} \geq 0$ for $n = 6, 7, 8, 9$. This means that $a_{i,i} \geq 0$ for $n \geq 6$ and for $2 \leq i \leq n-2$. As for $a_{i,n-2}$, we have:

$$\frac{\partial^2}{\partial i^2}((n-2)(i-1)a_{i,n-2}) = \frac{n-2}{4\sqrt{i^5}}(\frac{1}{\sqrt{n-1}} - \frac{i+3}{\sqrt{n-2}}) \leq 0$$

for $i \geq 2$. This means again that the function $(i-1)a_{i,n-2}$ is concave on i. Since $a_{2,n-2} = 0$ and $a_{n-2,n-2} \geq 0$, we conclude that $a_{i,n-2} \geq 0$ for $n \geq 6$ and $2 \leq i \leq n-2$. Finally, we obtain that $a_{i,j} \geq 0$ for $2 \leq i \leq n-2$ and $i \leq j \leq n-2$.

The function χ_1 attains minimum if we put $x_{2,j} = 0$ for $j = 2, 3, \ldots, n-3$ and $x_{i,j} = 0$ for $3 \leq i \leq n-2,\ i \leq j \leq n-2$. This minimum value is:

$$\bar{\chi}_1 = (\frac{n-3}{\sqrt{2(n-2)}} + \frac{n-3}{\sqrt{2(n-1)}} + \frac{1}{\sqrt{(n-2)(n-1)}})\frac{n-1}{n-2}$$

and $n_2 = n-2-\frac{1}{n-2},\ n_{n-2} = 1+\frac{1}{n-2},\ n_{n-1} = 1,\ n_i = 0$ for $i = 3, 4, \ldots, n-3$. This solution does not correspond to any graph, but the real graphical solution $\chi_1^* \geq \bar{\chi}_1$.

Now we show that $\bar{\chi}_1 \geq \chi_2^*$.

$$\begin{aligned}\bar{\chi}_1 - \chi_2^* &= \frac{1}{n-2}\left(\frac{n^2-4n+3}{\sqrt{2(n-2)}} - \frac{n^2-4n+5}{\sqrt{2(n-1)}} + \frac{n-1}{\sqrt{(n-2)(n-1)}} - \frac{n-2}{n-1}\right) \geq \\ & \frac{1}{n-2}\left(\frac{n^2-4n+3}{\sqrt{2(n-2)}} - \frac{n^2-4n+5}{\sqrt{2(n-1)}} + \frac{1}{n-1}\right) \geq 0\end{aligned}$$

for $n \geq 6$, because $\frac{1}{\sqrt{n-2}} \geq \frac{1}{\sqrt{n-1}}$ and because $(n^2-4n+3)\sqrt{n-1} \geq (n^2-4n+5)\sqrt{n-2}$ for $n \geq 7$. (After squaring, the last inequality becomes $n^4 - 12n^3 + 46n^2 - 72n + 41 \geq 0$ for $n \geq 7$. For $n = 6$, $\bar{\chi}_1 - \chi_2^* \geq 0$ is verified by numerical checking.)

Case 3: $n_{n-1} = 0$. In this case constraints (A) and (B) become:

$$\begin{array}{ccccccc} 2x_{2,2}+ & x_{2,3}+ & x_{2,4}+ & \ldots & + & x_{2,n-2} = & 2n_2 \\ x_{2,3}+ & 2x_{3,3}+ & x_{3,4}+ & \ldots & + & x_{3,n-2} = & 3n_3 \\ x_{2,4}+ & x_{3,4}+ & 2x_{4,4}+ & \ldots & + & x_{4,n-2} = & 4n_4 \\ & & & \vdots & & & \\ x_{2,n-2}+ & x_{3,n-2}+ & x_{4,n-2}+ & \ldots & + & 2x_{n-2,n-2} = & (n-2)n_{n-2} \end{array} \qquad (A'')$$

and

$$n_2 + n_3 + n_4 + \ldots + n_{n-2} = n \qquad (B'')$$

Now we solve the next problem of linear programming: $\min \chi_0$ under constraints (A'') and (B''). The basic variables are n_i for $i = 2, 3, \ldots, n-2$ and $x_{2,n-2}$. We find n_i for $i = 3, 4, \ldots, n-3$ from constraints (A''):

$$n_i = \frac{x_{2,i} + \ldots + x_{i-1,i} + 2x_{i,i} + x_{i,i+1} + \ldots + x_{i,n-2}}{i} \qquad (6)$$

Using the first and the last constraint of (A'') and constraint (B'') we find:

$$n_2 = n - 2 + \frac{2x_{2,2}}{n} - \sum_{j=3}^{n-3} \frac{n-j-2}{nj} x_{2,n-3} - \sum_{\substack{3\leq i\leq n-2 \\ i\leq j\leq n-2}} \left(\frac{n-2}{i} + \frac{n-2}{j}\right)\frac{x_{i,j}}{n}, \qquad (7)$$

$$n_{n-2} = 2 - \sum_{\substack{2\leq i\leq n-3 \\ i\leq j\leq n-3}} \left(\frac{2}{i} + \frac{2}{j}\right)\frac{x_{i,j}}{n} - \sum_{i=3}^{n-3}\left(\frac{2}{i} - 1\right)\frac{x_{i,n-2}}{n} - \frac{2x_{n-2,n-2}}{n}, \qquad (8)$$

$$x_{2,n-2} = 2(n-2) - \sum_{j=2}^{n-3} \frac{(j+2)(n-2)}{jn} x_{2,j} - 2\sum_{\substack{3\leq i\leq n-2 \\ i\leq j\leq n-2}} \left(\frac{n-2}{i} + \frac{n-2}{j}\right)\frac{x_{i,j}}{n} \qquad (9)$$

After substitution of $x_{2,n-2}$ from (9) into χ_0, we have:

$$\chi_0 = \frac{2(n-2)}{\sqrt{2(n-2)}} + \sum_{j=2}^{n-3} b_{2,j}x_{2,j} + \sum_{\substack{3\le i\le n-2\\ i\le j\le n-2}} b_{i,j}x_{i,j}$$

where

$$b_{i,j} = \frac{1}{\sqrt{ij}} - \frac{\frac{2(n-2)}{n}(\frac{1}{i}+\frac{1}{j})}{\sqrt{2(n-2)}}$$

We prove that all functions $b_{i,j} \ge 0$ for $2 \le i \le n-2,\ i \le j \le n-2$. Since

$$\frac{\partial b_{i,j}}{\partial j} = \frac{1}{2\sqrt{j^3}}(-\frac{1}{\sqrt{i}} + \frac{\sqrt{8(n-2)}}{n\sqrt{j}}) \le \frac{1}{2\sqrt{ij^3}}(-1 + \frac{\sqrt{8(n-2)}}{n}) \le 0$$

because $j \ge i$ and $-1 + \frac{\sqrt{8(n-2)}}{n} \le 0$ for $n \ge 4$, we have $b_{i,j} \ge b_{i,n-2}$.

$$b_{i,n-2} = \frac{1}{\sqrt{i(n-2)}}(1 - \frac{\sqrt{2}(n-2+i)}{n\sqrt{i}}) \ge 0$$

because $1 \ge \frac{\sqrt{2}(n-2+i)}{n\sqrt{i}}$ for $2 \le i \le n-2$. (After squaring, the last inequality becomes equivalent to $(i-2)((n-2)^2 - 2i) \ge 0$.)

Since all $a_{i,j} \ge 0$, the function χ_0 attains minimum if all $x_{2,j} = 0$ for $2 \le j \le n-3$, $x_{i,j} = 0$ for $3 \le i \le n-2, i \le j \le n-2$ and:

$$\chi_0^* = \frac{2(n-2)}{\sqrt{2(n-2)}}$$

We show that $\chi_0^* \ge \chi_2^*$:

$$\chi_0^* - \chi_2^* = \frac{1}{\sqrt{n-1}}(\frac{\sqrt{2(n-2)}}{\sqrt{n-2}+\sqrt{n-1}} - \frac{1}{\sqrt{n-1}} \ge \frac{1}{n-1}(\frac{\sqrt{2(n-2)}}{2} - 1) \ge 0$$

because $\frac{1}{\sqrt{n-2}} \ge \frac{1}{\sqrt{n-1}}$ and $\sqrt{2(n-2)} \ge 2$ for $n \ge 4$.

Finally we proved Theorem 1., that is, χ_2^* is minimum value of the Randić index and the extremal graph must have $n_2 = n-2,\ n_3 = n_4 = \ldots = n_{n-2} = 0,\ n_{n-1} = 2,\ x_{2,n-1} = 2(n-2)$, and all other $x_{i,j} = 0$. We proved this Theorem for $n \ge 6$, but numerical checking shows that it is true also for $n = 5$. □

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