ROMANIAN JOURNAL OF INFORMATION SCIENCE AND TECHNOLOGY
Volume **12**, Number 4, 2009, 455–465

On Dense Graphs Having Minimum Randić Index

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Abstract. In this paper all graphs G of order n and minimum degree $\delta(G) = k$ having minimum Randić index $R(G)$ are determined for $k \geq \lfloor n/2 \rfloor$. Each extremal graph is the join between a regular graph of order $n - s$ and a complete graph of order s (where $s \in \{n/2, (n+2)/2, (n-2)/2\}$ for n even and $s \in \{(n+1)/2, (n-1)/2\}$ for n odd). This yields an alternative proof in the case of dense graphs to that proposed by Li, Liu and Liu [5] who very recently solved a long-standing conjecture on Randić index. Also, the minimum value of this index in the class of graphs of order n and $\delta(G) = k$ is determined for $k \geq (n-1)/2$.

Key words: Randić index; complete graph; regular graph; non-linear programming model; graph join.

1. Introduction

The Randić index $R(G)$ of a graph G without isolated vertices was introduced in 1975 by Milan Randić under the name of "branching index" [9] as follows:

$$R(G) = \sum_{uv \in E(G)} (d(u)d(v))^{-1/2},$$

where $d(x)$ denotes the degree of a vertex $x \in V(G)$. The Randić index is also called "Randić connectivity index" or "connectivity index" [10].

Randić proposed this index in order to quantitatively characterize the degree of branching of the molecular skeleton, which is a critical factor for some physico-chemical properties of alcanes. Let $G(n,k)$ be the set of graphs without loops or multiple edges having n vertices and the minimum degree $\delta(G) = k$; the maximum degree will be denoted by $\Delta(G)$.

Fajtlowicz mentioned [4] that Bollobás and Erdös asked for the minimum value of the Randić index for graphs $G \in G(n,k)$. The solution of this problem turned out to be difficult.

For two vertex disjoint graphs, G and H, let $G + H$ denote their join, i. e., the graph obtained by joining by edges every vertex of G with all vertices of H; we shall also denote by $\overline{K_n}$ the complement of K_n, which consists of n isolated vertices.

In [2] Bollobás and Erdös solved the problem for $k = 1$ and proved that the extremal graph is unique and it coincides to $K_{1,n-1} = \overline{K_{n-1}} + K_1$; for $k = 2$ the problem was settled in [3] and the extremal graph is $\overline{K_{n-2}} + K_2$. Delorme, Favaron and Rautenbach also gave a conjecture about this problem in [3]:
In the set of graphs G of order n with $\delta(G) \geq k$ the unique extremal graph is $\overline{K_{n-k}} + K_k$; this conjecture is valid only for $k \leq n/2$ (see also [1]). Pavlović [7] using a quadratic programming approach and Kuhn-Tucker theorem showed that in the class $G(n, \lfloor n/2 \rfloor)$ the unique extremal graph is $\overline{K_{n-\lfloor n/2 \rfloor}} + K_{\lfloor n/2 \rfloor}$.

In this paper, using the quadratic programming model for this problem proposed by Pavlović and Divnić [8] and discrete optimization methods it is shown that every extremal graph in the class $G(n,k)$ is the join between a regular graph and a complete graph (of order $n/2, (n+2)/2$ or $(n-2)/2$ for n even and $(n+1)/2$ or $(n-1)/2$ for n odd) for every $k \geq \lfloor n/2 \rfloor$. These extremal graphs agree with the graphs found by Li, Liu and Liu [5] who determined by a different method all extremal graphs in $G(n,k)$ for $1 \leq k \leq n-1$.

2. Nonlinear programming model of Pavlović and Divnić

For a graph G of order n without loops or multiple edges denote by $\delta = \delta(G)$, $\Delta = \Delta(G)$, n_i the number of vertices of degree i for $\delta \leq i \leq \Delta$ ($n_\delta + n_{\delta+1} + \ldots + n_\Delta = n$) and by $x_{i,j} \geq 0$ the number of edges joining the vertices of degrees i and j ($\delta \leq i, j \leq \Delta$). Then

$$R(G) = \sum_{\delta \leq i \leq j \leq \Delta} \frac{x_{i,j}}{\sqrt{ij}}$$

and $\sum_{\substack{j=\delta \\ j \neq i}}^{\Delta} x_{i,j} + 2x_{i,i} = in_i$ for $\delta \leq i \leq \Delta$; $x_{i,j} \leq n_i n_j$ for $\delta \leq i < j \leq \Delta$; $x_{i,i} \leq \binom{n_i}{2}$ for $\delta \leq i \leq \Delta$; $x_{i,j} = x_{j,i}$ are nonnegative integers for $\delta \leq i \leq j \leq \Delta$.

We can associate to the problem of minimizing $R(G)$ the following nonlinear minimization problem:

$$\min r(x_{\delta,\delta}, \ldots, x_{\Delta,\Delta}) = \sum_{\delta \leq i \leq j \leq \Delta} \frac{x_{i,j}}{\sqrt{ij}}$$

subject to

$$\sum_{\substack{j=\delta\\ j\neq i}}^{\Delta} x_{i,j} + 2x_{i,i} = iz_i \text{ for } \delta \le i \le \Delta;$$

$$z_\delta + z_{\delta+1} + \ldots + z_\Delta = n; \tag{1}$$

$$x_{i,j} \le z_i z_j \text{ for } \delta \le i < j \le \Delta;$$

$$x_{i,i} \le \binom{z_i}{2} \text{ for } \delta \le i \le \Delta;$$

$$x_{i,j} = x_{j,i} \text{ and } z_i \text{ are nonnegative integers for } \delta \le i \le j \le \Delta.$$

Function r can also be written as [8]:

$$r(x_{\delta,\delta}, \ldots, x_{\Delta,\Delta}) = \frac{n}{2} - \frac{1}{2} \sum_{\delta \le i < j \le \Delta} \left(\frac{1}{\sqrt{i}} - \frac{1}{\sqrt{j}} \right)^2 x_{i,j}.$$

The problem of minimization of r becomes the problem of maximization of

$$\gamma(x_{\delta,\delta+1}, \ldots, x_{\Delta-1,\Delta}) = \sum_{\delta \le i < j \le \Delta} \left(\frac{1}{\sqrt{i}} - \frac{1}{\sqrt{j}} \right)^2 x_{i,j}.$$

By denoting $y_{i,j} = z_i z_j - x_{i,j}$ for $\delta \le i < j \le \Delta$ and $y_{i,i} = \binom{z_i}{2} - x_{i,i}$ for $\delta \le i \le \Delta$ we get

$$\gamma(x_{\delta,\delta+1}, \ldots, x_{\Delta-1,\Delta}) = \gamma_1(z_\delta, \ldots, z_\Delta) + \gamma_2(y_{\delta,\delta+1}, \ldots, y_{\Delta-1,\Delta}),$$

where $\gamma_1 = \sum_{\delta \le i < j \le \Delta} \left(\frac{1}{\sqrt{i}} - \frac{1}{\sqrt{j}} \right)^2 z_i z_j$ and $\gamma_2 = -\sum_{\delta \le i < j \le \Delta} \left(\frac{1}{\sqrt{i}} - \frac{1}{\sqrt{j}} \right)^2 y_{i,j}$.

We have $y_{i,j} \ge 0$ for $\delta \le i < j \le \Delta$; $y_{i,i} \ge 0$ for $\delta \le i \le \Delta$ and $y_{i,j} = y_{j,i}$ are integers for $\delta \le i \le j \le \Delta$. It is clear that

$$\max \gamma \le \max \gamma_1 + \max \gamma_2.$$

We have $\max \gamma_2 = 0$ and this holds if and only if $y_{i,j} = 0$ for $\delta \le i < j \le \Delta$, or equivalently, $x_{i,j} = z_i z_j$ for all indices $\delta \le i < j \le \Delta$.

In the next section we shall consider the problem of maximizing γ_1 and all sequences $(z_\delta, \ldots, z_\Delta)$ reaching the first and the second maximum values of γ_1 will be found. These sequences which have graphical realizations also reach the maximum of γ_2, hence the maximum of γ.

3. A technical lemma

Denote $\varphi(n) = \max_{\substack{n_1+n_2=n \\ n_1,n_2\in \mathbb{Z}}} n_1 n_2$; it follows that $\varphi(n) = n^2/4$ for n even ($n_1 = n_2 = n/2$) and $\varphi(n) = (n^2-1)/4$ for n odd ($\{n_1, n_2\} = \{(n-1)/2, (n+1)/2\}$). If $1 \le \delta < \Delta \le n-1$, $\delta, \Delta \in \mathbb{N}$, consider the function

$$f(x_\delta, x_{\delta+1}, \ldots, x_\Delta) = \sum_{\delta \le i < j \le \Delta} \left(\frac{1}{\sqrt{i}} - \frac{1}{\sqrt{j}} \right)^2 x_i x_j$$

and the domains $D = \{(x_\delta, x_{\delta+1}, \ldots, x_\Delta) : x_i \in \mathbb{N} \text{ for } \delta \le i \le \Delta, \sum_{i=\delta}^{\Delta} x_i = n\}$; $D_1 = D \backslash \{(n/2, 0, \ldots, 0, n/2)\}$ for n even and $D_1 = D \backslash \{((n-1)/2, 0, \ldots, 0, (n+1)/2), ((n+1)/2, 0, \ldots, 0, (n-1)/2)\}$ for n odd.

Lemma 3.1. *All points where f is maximum in D and D_1, respectively, are the following: i) If $n \ge 4$ is even, then $\max_D f(x_\delta, \ldots, x_\Delta)$ is reached for $(n/2, 0, \ldots, 0, n/2)$ and $\max_{D_1} f(x_\delta, \ldots, x_\Delta)$ for $((n-2)/2, 0, \ldots, 0, (n+2)/2)$ and $((n+2)/2, 0, \ldots, 0, (n-2)/2)$; ii) If $n \ge 5$ is odd, then $\max_D f(x_\delta, \ldots, x_\Delta)$ is attained for $((n-1)/2, 0, \ldots, 0, (n+1)/2)$ and $((n+1)/2, 0, \ldots, 0, (n-1)/2)$ and $\max_{D_1} f(x_\delta, \ldots, x_\Delta)$ when $(x_\delta, \ldots x_\Delta)$ is located into the set $\{((n-3)/2, 0, \ldots, 0, (n+3)/2), ((n+3)/2, 0, \ldots, 0, (n-3)/2), ((n-1)/2, 0, \ldots, 0, 1, (n-1)/2)\}$.*

Proof. **A.** First we shall determine the maximum of $f(x_\delta, \ldots, x_\Delta)$ when $(x_\delta, \ldots, x_\Delta) \in D$. If $x_{\delta+1} = \ldots = x_{\Delta-1} = 0$ then

$$f(x_\delta, \ldots, x_\Delta) = \left(\frac{1}{\sqrt{\delta}} - \frac{1}{\sqrt{\Delta}} \right)^2 x_\delta x_\Delta,$$

and the result is obvious since $x_\delta + x_\Delta = n$.

Otherwise, denote by $i\,(\delta+1 \le i \le \Delta-1)$ the smallest index such that $x_i \ge 1$ and by $j\,(\delta+1 \le j \le \Delta-1)$ the greatest index such that $x_j \ge 1$; obviously $i \le j$. Denote by α and β the operations consisting of replacing $x = (x_\delta, \ldots, x_\Delta) \in D$ by $x' = (x_\delta, 0, \ldots, 0, x_i, \ldots, x_{j-1}, x_j - 1, 0, \ldots, 0, x_\Delta + 1) \in D$ and by $x'' = (x_\delta + 1, 0, \ldots, 0, x_i - 1, x_{i+1}, \ldots, x_j, 0, \ldots, 0, x_\Delta) \in D$, respectively. We have:

$$f(x') - f(x) = \left(\frac{1}{\sqrt{j}} - \frac{1}{\sqrt{\Delta}} \right)^2 (x_j - x_\Delta - 1) + x_\delta \left(\frac{1}{\sqrt{j}} - \frac{1}{\sqrt{\Delta}} \right) \left(\frac{2}{\sqrt{\delta}} - \frac{1}{\sqrt{j}} - \frac{1}{\sqrt{\Delta}} \right)$$
$$+ x_i \left(\frac{1}{\sqrt{j}} - \frac{1}{\sqrt{\Delta}} \right) \left(\frac{2}{\sqrt{i}} - \frac{1}{\sqrt{j}} - \frac{1}{\sqrt{\Delta}} \right) + x_{i+1} \left(\frac{1}{\sqrt{j}} - \frac{1}{\sqrt{\Delta}} \right) \left(\frac{2}{\sqrt{i+1}} - \frac{1}{\sqrt{j}} - \frac{1}{\sqrt{\Delta}} \right) +$$
$$\ldots + x_{j-1} \left(\frac{1}{\sqrt{j}} - \frac{1}{\sqrt{\Delta}} \right) \left(\frac{2}{\sqrt{j-1}} - \frac{1}{\sqrt{j}} - \frac{1}{\sqrt{\Delta}} \right).$$

Since $\dfrac{2}{\sqrt{k}} - \dfrac{1}{\sqrt{j}} - \dfrac{1}{\sqrt{\Delta}} > \dfrac{1}{\sqrt{j}} - \dfrac{1}{\sqrt{\Delta}}$ for $k = \delta, i, i+1, \ldots, j-1$, we can write

$$f(x') - f(x) \ge \left(\frac{1}{\sqrt{j}} - \frac{1}{\sqrt{\Delta}} \right)^2 (x_\delta + x_i + x_{i+1} + \ldots + x_j - x_\Delta - 1) \qquad (2)$$

and this inequality is strict if at least one of $x_\delta, x_i, x_{i+1}, \ldots, x_{j-1}$ is different from zero. Similarly,

$$f(x'')-f(x) = \left(\frac{1}{\sqrt{\delta}} - \frac{1}{\sqrt{i}}\right)^2 (x_i - x_\delta - 1) + x_{i+1}\left(\frac{1}{\sqrt{\delta}} - \frac{1}{\sqrt{i}}\right)\left(\frac{1}{\sqrt{\delta}} + \frac{1}{\sqrt{i}} - \frac{2}{\sqrt{i+1}}\right) +$$

$$\ldots + x_j\left(\frac{1}{\sqrt{\delta}} - \frac{1}{\sqrt{i}}\right)\left(\frac{1}{\sqrt{\delta}} + \frac{1}{\sqrt{i}} - \frac{2}{\sqrt{j}}\right) + x_\Delta\left(\frac{1}{\sqrt{\delta}} - \frac{1}{\sqrt{i}}\right)\left(\frac{1}{\sqrt{\delta}} + \frac{1}{\sqrt{i}} - \frac{2}{\sqrt{\Delta}}\right),$$

which implies:

$$f(x'') - f(x) \geq \left(\frac{1}{\sqrt{\delta}} - \frac{1}{\sqrt{i}}\right)^2 (x_i + x_{i+1} + \ldots + x_j + x_\Delta - x_\delta - 1) \tag{3}$$

and this inequality is strict if at least one of $x_{i+1}, \ldots, x_j, x_\Delta$ is different from zero.

If $i = j$ we get

$$f(x') - f(x) \geq \left(\frac{1}{\sqrt{i}} - \frac{1}{\sqrt{\Delta}}\right)^2 (x_\delta + x_i - x_\Delta - 1), \tag{4}$$

the inequality being strict if $x_\delta \geq 1$ and

$$f(x'') - f(x) \geq \left(\frac{1}{\sqrt{\delta}} - \frac{1}{\sqrt{i}}\right)^2 (x_\Delta + x_i - x_\delta - 1), \tag{5}$$

and this inequality is strict if $x_\Delta \geq 1$.

We shall prove that at least one of the differences $f(x') - f(x)$ and $f(x'') - f(x)$ is greater than zero, which implies that all sequences $(x_\delta, \ldots, x_\Delta) \in D$ realizing maximum of f satisfy $x_{\delta+1} = \ldots = x_{\Delta-1} = 0$. Consider first the case when $i = j$. It is clear that if $x_\delta = x_\Delta = 0$ then $f(x_\delta, \ldots, x_\Delta) = 0$ which implies that $(0, \ldots, 0, x_i, 0, \ldots, 0)$ cannot maximize f. Otherwise, suppose that $x_\delta \geq 1$. If $x_\delta + x_i - x_\Delta - 1 \geq 0$ then (4) is strict and it follows that $f(x') > f(x)$ and x cannot maximize f on D. Otherwise, $x_\delta + x_i - x_\Delta - 1 \leq -1$. In this case $x_\Delta \geq x_\delta + x_i$, hence $x_\Delta + x_i - x_\delta - 1 \geq 2x_i - 1 \geq 1$, which implies $f(x'') > f(x)$ and x also cannot maximize f. If $x_\Delta \geq 1$ the same conclusion follows since (5) is strict.

Suppose that $i < j$. In this case $x_i > 0, x_j > 0$ and both inequalities (2) and (3) are strict. If $x_\delta + x_i + \ldots + x_j - x_\Delta - 1 \geq 0$ then from (2) it follows that $f(x') > f(x)$. Otherwise, $x_\Delta \geq x_\delta + x_i + \ldots + x_j$ and $x_i + \ldots + x_j + x_\Delta - x_\delta - 1 \geq 2(x_i + \ldots + x_j) - 1 > 0$, which implies $f(x'') > f(x)$ from (3).

Consequently, all sequences maximizing f have the form $(n_1, 0, \ldots, 0, n_2)$, where $n_1 + n_2 = n$; in this case

$$f(n_1, 0, \ldots, 0, n_2) = \left(\frac{1}{\sqrt{\delta}} - \frac{1}{\sqrt{\Delta}}\right)^2 n_1 n_2 \leq \left(\frac{1}{\sqrt{\delta}} - \frac{1}{\sqrt{\Delta}}\right)^2 \varphi(n)$$

and the conclusion follows.

B. Consider that $x = (x_\delta, \ldots, x_\Delta) \in D_1$. If $x_{\delta+1} = \ldots = x_{\Delta-1} = 0$ then $f(x_\delta, \ldots, x_\Delta) = \left(\frac{1}{\sqrt{\delta}} - \frac{1}{\sqrt{\Delta}}\right)^2 x_\delta x_\Delta$, where $x_\delta + x_\Delta = n$ and the result is obvious.

If $x_{\delta+1} + \ldots + x_{\Delta-1} \geq 2$ then we have seen that by an operation α or β we can find sequences $y, z \in D$ such that $f(x) < f(y) < f(z)$, hence x cannot maximize f on D_1. If $x_{\delta+1} + \ldots + x_{\Delta-1} = 1$ we shall consider other two subcases: B1: n is even; B2: n is odd.

B1. If n is even we shall prove that x cannot maximize f if $x_{\delta+1}+\ldots+x_{\Delta-1} = 1$, i.e., there exists an index $i, \delta + 1 \leq i \leq \Delta - 1$ such that $x_i = 1$ and $x_j = 0$ for every $\delta + 1 \leq j \leq \Delta - 1$ and $j \neq i$.

Let $k = \min(x_\delta, x_\Delta) \leq n/2 - 1$. Without loss of generality suppose that $k = x_\delta$. If $k = n/2 - 1$, then $x_\delta = n/2 - 1$ and $x_\Delta = n/2$. Applying transformation α we deduce that

$$f(n/2-1,0,\ldots,0,n/2+1) - f(n/2-1,0,\ldots,0,1,0,\ldots,0,n/2) =$$

$$\left(\frac{n}{2}-1\right)\left(\frac{2}{\sqrt{\delta}}-\frac{1}{\sqrt{i}}-\frac{1}{\sqrt{\Delta}}\right)\left(\frac{1}{\sqrt{i}}-\frac{1}{\sqrt{\Delta}}\right)-\frac{n}{2}\left(\frac{1}{\sqrt{i}}-\frac{1}{\sqrt{\Delta}}\right)^2 =$$

$$\left(\frac{1}{\sqrt{i}}-\frac{1}{\sqrt{\Delta}}\right)\left(\frac{n-2}{\sqrt{\delta}}-\frac{n-1}{\sqrt{i}}+\frac{1}{\sqrt{\Delta}}\right).$$

We shall prove that

$$\frac{n-2}{\sqrt{\delta}}-\frac{n-1}{\sqrt{i}}+\frac{1}{\sqrt{\Delta}} > 0, \tag{6}$$

which will prove that $(n/2-1,0,\ldots,0,1,0,\ldots,0,n/2)$ cannot maximize f on D_1. We have

$$\frac{n-2}{\sqrt{\delta}}-\frac{n-1}{\sqrt{i}}+\frac{1}{\sqrt{\Delta}} \geq \frac{n-2}{\sqrt{\delta}}-\frac{n-1}{\sqrt{\delta+1}}+\frac{1}{\sqrt{n-1}}.$$

Consider now the function $g(x) = \dfrac{n-2}{\sqrt{x}} - \dfrac{n-1}{\sqrt{x+1}}$, where $x \in [1, n-3]$. Its derivative $g'(x) = \dfrac{1}{2}(\dfrac{n-1}{(x+1)\sqrt{x+1}} - \dfrac{n-2}{x\sqrt{x}})$ is negative since this is equivalent to $x^3(n-1)^2 < (x+1)^3(n-2)^2$, or

$$x^2(x(2n-3)-3(n-2)^2)-3(n-2)^2x-(n-2)^2 < 0. \tag{7}$$

We deduce that $x(2n-3) < 3(n-2)^2$ for $x \leq n-3$ since $n-3 < 3(n-2)^2/(2n-3)$ is equivalent to $n^2 - 3n + 3 > 0$ and this holds for $n \geq 4$. It follows that (7) is true, which implies that g is strictly decreasing on the interval $[1, n-3]$. We get $\dfrac{n-2}{\sqrt{\delta}} - \dfrac{n-1}{\sqrt{\delta+1}} + \dfrac{1}{\sqrt{n-1}} \geq \dfrac{n-2}{\sqrt{n-3}} - \dfrac{n-1}{\sqrt{n-2}} + \dfrac{1}{\sqrt{n-1}}$. It remains to show that

$$\frac{n-2}{\sqrt{n-3}}-\frac{n-1}{\sqrt{n-2}}+\frac{1}{\sqrt{n-1}} > 0 \tag{8}$$

for every $n \geq 4$. By elementary calculation we deduce that (8) is equivalent to $2(n-2)^2\sqrt{(n-1)(n-3)} > n^3 - 7n^2 + 15n - 11$ for every $n \geq 4$. But $2(n-2)^2\sqrt{(n-1)(n-3)} > 2(n-2)^2(n-3) > n^3 - 7n^2 + 15n - 11$ since the last inequality is equivalent to $n^3 - 7n^2 + 17n - 13 > 0$, which is true for $n \geq 4$. Consequently, (6) is true for every $1 \leq \delta < i < \Delta \leq n-1$ and $n \geq 4$.

If $k = x_\delta \leq n/2 - 2$ it follows that $x_\Delta \geq n/2 + 1$ and applying a transformation β we deduce from (5) that $f(x_\delta + 1, 0, \ldots, 0, x_\Delta) - f(x_\delta, 0, \ldots, 0, 1, 0, \ldots, 0, x_\Delta) > 3\left(\frac{1}{\sqrt{\delta}} - \frac{1}{\sqrt{i}}\right)^2 > 0$ since $x_\Delta - x_\delta \geq 3$. In this case $f(x_\delta + 1, 0, \ldots, 0, x_\Delta) \leq \left(\frac{1}{\sqrt{\delta}} - \frac{1}{\sqrt{\Delta}}\right)^2 (n/2-1)(n/2+1) < \max_D f$, which implies that $(x_\delta, \ldots, x_\Delta)$ cannot maximize f on D_1. If $\min(x_\delta, x_\Delta) = x_\Delta$ we deduce that only $(n/2+1, 0, \ldots, 0, n/2-1)$ maximize f on D_1.

B2. If n is odd and $\min(x_\delta, x_\Delta) = x_\delta$ it follows that $x_\delta \leq (n-1)/2$. If $x_\delta = (n-1)/2$ and $x_i = 1$ we get $x_\Delta = (n-1)/2$ and

$$f((n-1)/2, 0, \ldots, 0, 1, 0, \ldots, 0, (n-1)/2) =$$

$$\left(\frac{1}{\sqrt{\delta}} - \frac{1}{\sqrt{\Delta}}\right)^2 \left(\frac{n-1}{2}\right)^2 + \left(\frac{1}{\sqrt{\delta}} - \frac{1}{\sqrt{i}}\right)^2 \frac{n-1}{2} + \left(\frac{1}{\sqrt{i}} - \frac{1}{\sqrt{\Delta}}\right)^2 \frac{n-1}{2} =$$

$$\left(\frac{1}{\sqrt{\delta}} - \frac{1}{\sqrt{\Delta}}\right)^2 \left(\frac{n-1}{2}\right)^2 + \left(\frac{1}{\delta} + \frac{1}{\Delta}\right) \frac{n-1}{2} + (n-1)h(i),$$

where

$$h(i) = \frac{1}{i} - \frac{C}{\sqrt{i}} \tag{9}$$

and $C = \frac{1}{\sqrt{\delta}} + \frac{1}{\sqrt{\Delta}}$. By considering the function $g(x) = \frac{1}{x} - \frac{C}{\sqrt{x}}$ defined on the interval (δ, Δ), we get $g'(x) = \frac{C\sqrt{x} - 2}{2x^2}$ having a unique root $x_0 = 4/C^2$. Since $\frac{2}{\sqrt{\Delta}} < C < \frac{2}{\sqrt{\delta}}$ it follows that $x_0 \in (\delta, \Delta)$ and $g(x)$ is decreasing on (δ, x_0) and increasing on (x_0, Δ). Therefore

$$\max_{\delta+1 \leq i \leq \Delta-1} h(i) = \max\left(h(\delta+1), h(\Delta-1)\right) = h(\Delta-1) =$$

$$\frac{1}{\Delta-1} - \left(\frac{1}{\sqrt{\delta}} + \frac{1}{\sqrt{\Delta}}\right) \frac{1}{\sqrt{\Delta-1}}, \text{ since}$$

$$0 > \frac{1}{\sqrt{\delta+1}} - \left(\frac{1}{\sqrt{\delta}} + \frac{1}{\sqrt{\Delta}}\right) > \frac{1}{\sqrt{\Delta-1}} - \left(\frac{1}{\sqrt{\delta}} + \frac{1}{\sqrt{\Delta}}\right) \text{ and } \frac{1}{\sqrt{\delta+1}} > \frac{1}{\sqrt{\Delta-1}}.$$

It follows that

$$\frac{1}{\sqrt{\delta+1}}\left(\frac{1}{\sqrt{\delta+1}} - \left(\frac{1}{\sqrt{\delta}} + \frac{1}{\sqrt{\Delta}}\right)\right) < \frac{1}{\sqrt{\Delta-1}}\left(\frac{1}{\sqrt{\Delta-1}} - \left(\frac{1}{\sqrt{\delta}} + \frac{1}{\sqrt{\Delta}}\right)\right).$$

Hence in the set of all sequences $(x_\delta, \ldots, x_\Delta) \in D_1$ such that $x_\delta = x_\Delta = (n-1)/2$ and $x_{\delta+1} + \ldots + x_{\Delta-1} = 1$ the maximum of f is reached only for $x_{\delta+1} = \ldots = x_{\Delta-2} = 0$ and $x_{\Delta-1} = 1$.

If $x_\delta = \min(x_\delta, x_\Delta) = (n-3)/2$, $x_i = 1$ and $x_j = 0$ for every $\delta+1 \le j \le \Delta-1, j \ne i$ we deduce $x_\Delta = (n+1)/2$ and $f((n-1)/2, 0, \ldots, 0, 1, 0, \ldots, 0, (n-1)/2) - f((n-3)/2, 0, \ldots, 0, 1, 0, \ldots, 0, (n+1)/2) = 2\left(\frac{1}{\sqrt{\delta}} - \frac{1}{\sqrt{i}}\right)\left(\frac{1}{\sqrt{\delta}} - \frac{1}{\sqrt{\Delta}}\right) > 0$, both sequences having a unity on the same position i. If $x_\Delta = \min(x_\delta, x_\Delta) = (n-3)/2$ we also obtain $f((n-1)/2, 0, \ldots, 0, 1, 0, \ldots, 0, (n-1)/2) - f((n+1)/2, 0, \ldots, 0, 1, 0, \ldots, 0, (n-3)/2) = 2\left(\frac{1}{\sqrt{\delta}} - \frac{1}{\sqrt{\Delta}}\right)\left(\frac{1}{\sqrt{i}} - \frac{1}{\sqrt{\Delta}}\right) > 0$. Otherwise $\min(x_\delta, x_\Delta) \le (n-5)/2$ and we deduce as for n even that $(x_\delta, \ldots, x_\Delta)$ cannot maximize f on D_1. Also, if $x_{\delta+1} = \ldots = x_{\Delta-1} = 0$ then maximum of f on D_1 is reached for $((n-3)/2, 0, \ldots, 0, (n+3)/2)$ or for $((n+3)/2, 0, \ldots, 0, (n-3)/2)$ and the proof is complete. ☐

Corollary 3.2. *If $\delta = k, x_k = n-k+t, k \le n/2, 0 \le t \le k$, then $\max_D f(x_k, \ldots, x_{n-1})$ is reached only for $(n-k+t, 0, \ldots, 0, k-t)$.*

Proof. Let $\Delta = n-1$ and suppose that $x = (x_k, \ldots, x_{n-1}) \in D$ realizes $\max_D f$. From the hypothesis it follows that $x_k \ge n/2 + t \ge n/2$. If there exists at least an index $i, k+1 \le i \le n-2$ such that $x_i \ge 1$, by applying operation α we can get another sequence x' such that $f(x') - f(x) > 0$ by (2) or (4) since $x_{n-1} < n/2$, a contradiction. ☐

This result is also deduced in [8, Theorem 1] by using Kuhn-Tucker theorem.

4. Main results

A conjecture proposed in [3] (and amended in [1]) asserts that if G is a graph of order n satisfying $\delta(G) \ge k$, then $R(G)$ is minimum if and only if $G = \overline{K_{n-k}} + K_k$. We shall prove that every graph $G \in G(n, k)$ having $R(G)$ minimum is a join between a regular graph and a complete graph for every $k \ge \lfloor n/2 \rfloor$.
Let $\mathcal{H}(n, r)$ be the set of graphs of order n which are r-regular. $\mathcal{H}(n, r) \ne \emptyset$ if and only if $r \le n-1$ and nr is even (see for example [6]).

Theorem 4.1. *Let G be a graph of order n and $\delta(G) = k \ge \lfloor n/2 \rfloor$. If its Randić index is minimum, then G is a join between a regular graph and a complete graph, namely:*
i) *If n is even, then:*
$G = H + K_{n/2}$, *where* $H \in \mathcal{H}(n/2, k - n/2)$ *for k even and* $n \equiv 0 \pmod 4$, *k odd and* $n \equiv 0 \pmod 4$, *k odd and* $n \equiv 2 \pmod 4$*;*
$G = H + K_{(n+2)/2}$, *where* $H \in \mathcal{H}((n-2)/2, k - (n+2)/2)$ *if* $k \ge (n+2)/2$ *for k even and* $n \equiv 2 \pmod 4$ *or*
$G = H + K_{(n-2)/2}$, *where* $H \in \mathcal{H}((n+2)/2, k - (n-2)/2)$ *for k even and* $n \equiv 2 \pmod 4$.
ii) *If n is odd, then:*
$G = H + K_{(n+1)/2}$, *where* $H \in \mathcal{H}((n-1)/2, k - (n+1)/2)$ *if* $k \ge (n+1)/2$ *for k even and* $n \equiv 1 \pmod 4$, *k even and* $n \equiv 3 \pmod 4$, *k odd and* $n \equiv 1 \pmod 4$, *or*
$G = H + K_{(n-1)/2}$, *where* $H \in \mathcal{H}((n+1)/2, k - (n-1)/2)$ *for k even and* $n \equiv 1 \pmod 4$, *k even and* $n \equiv 3 \pmod 4$, *k odd and* $n \equiv 3 \pmod 4$.

Proof. i) If n is even, from Lemma 3.1 with $\delta = k$ and $\Delta = n-1$ we deduce that $\max \gamma_1$ is reached only for $(z_k, \ldots, z_{n-1}) = (n/2, 0, \ldots, 0, n/2)$. It follows that the vertices of degree $n-1$ induce a complete subgraph $K_{n/2}$ and the remaining vertices, of degree k, a subgraph which is regular of degree $k - n/2$. This subgraph exists only if $\frac{n}{2}(k - \frac{n}{2})$ is an even number, i.e., when k is even and $n \equiv 0 \pmod 4$, k is odd and $n \equiv 0 \pmod 4$ or when k is odd and $n \equiv 2 \pmod 4$. In these cases any extremal graph is of the form $H + K_{n/2}$, where H belongs to $\mathcal{H}(n/2, k-n/2)$ since $\max \gamma_2 = 0$ ($x_{i,j} = z_i z_j$ for $n/2 \le i < j \le n-1$).

In the remaining case (k even and $n \equiv 2 \pmod 4$) there is no graphical realization for $(n/2, 0, \ldots, 0, n/2)$ and we shall consider the second maximum value for γ_1. This value is reached only for $x_1 = (n/2-1, 0, \ldots, 0, n/2+1)$ and $x_2 = (n/2+1, 0, \ldots, 0, n/2-1)$. In the case of x_1 we deduce that there exists a graphical realization, namely $H + K_{n/2+1}$, where $H \in \mathcal{H}(n/2-1, k-n/2-1)$ if $k \ge n/2+1$ and k is even and $n \equiv 2 \pmod 4$. In this case also $\max \gamma_2 = 0$, hence this second extremal value of γ_1 is also a second extremal value of γ. If the second extremal point is x_2, there also exists a graphical realization $H + K_{n/2-1}$, where $H \in \mathcal{H}(n/2+1, k-n/2+1)$ if k is even and $n \equiv 2 \pmod 4$.

Note that for $k = n/2$ it is not possible to have k even and $n \equiv 2 \pmod 4$, the extremal graph is only $\overline{K_{n/2}} + K_{n/2}$. This result was also deduced in [7].

ii) If n is odd then $\max \gamma_1$ is reached for $x_3 = ((n-1)/2, 0, \ldots, 0, (n+1)/2)$ or $x_4 = ((n+1)/2, 0, \ldots, 0, (n-1)/2)$. x_3 correspond to a graphical realization $H + K_{(n+1)/2}$, where $H \in \mathcal{H}((n-1)/2, k-(n+1)/2)$ if $k \ge (n+1)/2$ for k even and $n \equiv 1 \pmod 4$, k even and $n \equiv 3 \pmod 4$ or k odd and $n \equiv 1 \pmod 4$. For x_4 we obtain $H + K_{(n-1)/2}$, where $H \in \mathcal{H}((n+1)/2, k-(n-1)/2)$ if k is even and $n \equiv 1 \pmod 4$, k is even and $n \equiv 3 \pmod 4$ or k is odd and $n \equiv 3 \pmod 4$.

For $k = (n-1)/2$ it is not possible to have k odd and $n \equiv 1 \pmod 4$ and the extremal graph is unique and it coincides with $\overline{K_{(n+1)/2}} + K_{(n-1)/2}$ (see also [7]). Consequently, in all possible cases for k and n odd there exists at least one extremal graph in this list. Also, in all cases $x_{i,j} = z_i z_j$ for $(n-1)/2 \le i < j \le n-1$, which implies $\max \gamma_2 = 0$.

For n odd it was not necessary to consider the second maximum point of γ_1, which is more difficult to localize relatively to the case when n was even. □

Theorem 4.2. *If G is a graph of order n, n is even and $\delta(G) = n/2 - 1$, then $R(G)$ is minimum only if $G = \overline{K_{n/2+1}} + K_{n/2-1}$.*

Proof. By Lemma 3.1 $f(x_{n/2-1}, \ldots, x_{n-1})$ is maximum in D only for $x_{n/2-1} = n/2, x_{n/2} = \ldots = x_{n-2} = 0$ and $x_{n-1} = n/2$. This degree distribution has no graphical realization since in this case $x_{n-1} = n/2$ implies $\delta(G) \ge n/2$. This function has in D_1 two extremal points and one of them, namely $(n/2+1, 0, \ldots, 0, n/2-1)$ has a graphical realization, $\overline{K_{n/2+1}} + K_{n/2-1}$. Since $x_{i,j} = x_i x_j$ for $n/2-1 \le i < j \le n-1$ it follows that $\max \gamma_2 = 0$ and this graph is the single graph with a minimum Randić index in $G(n, n/2-1)$ when n is even. □

Denote by $F(n,k)$ the class of graphs G of order n without loops or multiple edges and $\delta(G) \ge k$, i.e., $F(n,k) = \bigcup_{k \le k' \le n-1} G(n,k')$. The problem of finding minimum

Randić index in this class of graphs, raised in [3], can be solved for every $k \geq \lfloor n/2 \rfloor$.

Corollary 4.3. i) *If* n *is odd and* $(n-1)/2 \leq k \leq n-1$ *then*

$$\min_{G \in F(n,k)} R(G) = \frac{n}{2} - \left(\frac{1}{\sqrt{k}} - \frac{1}{\sqrt{n-1}} \right)^2 (n^2-1)/8;$$

ii) *If* n *is even and* $n/2 - 1 \leq k \leq n-1$ *then*

$$\min_{G \in F(n,k)} R(G) = \begin{cases} \frac{n}{2} - \left(\frac{1}{\sqrt{k}} - \frac{1}{\sqrt{n-1}} \right)^2 n^2/8, & \textit{if } k \textit{ is even and } n \equiv 0 \pmod 4, \\ & k \textit{ is odd and } n \equiv 0 \pmod 4 \\ & \textit{or } k \textit{ is odd and } n \equiv 2 \pmod 4; \\ \frac{n}{2} - \left(\frac{1}{\sqrt{k}} - \frac{1}{\sqrt{n-1}} \right)^2 (n^2-4)/8, & \textit{if } k \textit{ even and } n \equiv 2 \pmod 4. \end{cases}$$

Proof. We have

$$\max_{k \leq k' \leq n-1} \left(\frac{1}{\sqrt{k'}} - \frac{1}{\sqrt{n-1}} \right)^2 = \left(\frac{1}{\sqrt{k}} - \frac{1}{\sqrt{n-1}} \right)^2 .$$

Also, if n is even, $n \equiv 2 \pmod 4$ and k is even, then $k+1$ is odd and it is necessary to show that

$$\left(\frac{1}{\sqrt{k}} - \frac{1}{\sqrt{n-1}} \right)^2 (n^2-4) > \left(\frac{1}{\sqrt{k+1}} - \frac{1}{\sqrt{n-1}} \right)^2 n^2. \tag{10}$$

(10) is equivalent to

$$\frac{n^2}{4} \left(\frac{1}{\sqrt{k}} - \frac{1}{\sqrt{k+1}} \right) \left(\frac{1}{\sqrt{k}} + \frac{1}{\sqrt{k+1}} - \frac{2}{\sqrt{n-1}} \right) > \left(\frac{1}{\sqrt{k}} - \frac{1}{\sqrt{n-1}} \right)^2 .$$

Since

$$\frac{1}{\sqrt{k}} + \frac{1}{\sqrt{k+1}} - \frac{2}{\sqrt{n-1}} \geq \frac{1}{\sqrt{k}} - \frac{1}{\sqrt{n-1}},$$

it is sufficient to show that

$$\frac{n^2}{4} \left(\frac{1}{\sqrt{k}} - \frac{1}{\sqrt{k+1}} \right) > \frac{1}{\sqrt{k}} - \frac{1}{\sqrt{n-1}}$$

for every $1 \leq k \leq n-2$. This property can be proved easily since function $f(k) = \frac{1}{\sqrt{k}} - \frac{1}{\sqrt{k+1}}$ is strictly decreasing on the interval $[1, n-2]$. □

Concluding remarks

Using an approach different from that of Pavlović and Divnić [7, 8] we have obtained more information about the extremal points of the function γ_1, which allowed us to characterize graphs of order n and minimum degree equal to k having minimum Randić index for every $\lfloor n/2 \rfloor \leq k \leq n-1$ and also for n even and $k = n/2 - 1$.
The conjecture attributed to Delorme, Favaron and Rautenbach in [7], namely the Randić index for graphs in $G(n,k)$, where $1 \leq k \leq n/2$ attains its minimum value only for $\overline{K_{n-k}} + K_k$, was solved by Li, Liu and Liu [5].

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