THE VARIATION OF THE RANDIĆ INDEX WITH REGARD TO MINIMUM AND MAXIMUM DEGREE

Milica Milivojević,Ljiljana Pavlović[1],

Faculty of Science and Mathematics, University of Kragujevac,
Radoja Domanovića 12, Kragujevac, Serbia.

Abstract. The variation of the Randić index $R'(G)$ of a graph G is defined by $R(G) = \sum_{uv\in E(G)} \frac{1}{\max\{d(u)d(v)\}}$, where $d(u)$ is the degree of vertex u and the summation extends over all edges uv of G. Let $G(k,n)$ be the set of connected simple n-vertex graphs with minimum vertex degree k. In this paper we found in $G(k,n)$ graphs for which the variation of the Randić index attains its minimum value. When $k \le \frac{n}{2}$ the extremal graphs are complete split graphs $K^*_{k,n-k}$, which have only vertices of two degrees, i.e. degree k and degree $n-1$, and the number of vertices of degree k is $n-k$, while the number of vertices of degree $n-1$ is k. For $k \ge \frac{n}{2}$ the extremal graphs have also vertices of two degrees k and $n-1$, and the number of vertices of degree k is $\frac{n}{2}$. Further, we generalized results for graphs with given maximum degree.

Keywords: Simple graphs with given minimum degree, Variation of the Randić index, Combinatorial optimization, Quadratic programming.

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1. INTRODUCTION

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 $R(G)$ of a graph G, defined in [13], is given by

$$R(G) = \sum_{uv\in E(G)} \frac{1}{\sqrt{d(u)d(v)}},$$

where the summation extends over all edges of G and $d(u)$ is the degree of the vertex u in G. Randić himself demonstrated [13] that this index is well correlated with a variety of physico-chemical properties of alkanes. The Randić index has become one of the most popular molecular descriptors. To this index several books are devoted ([8-10]). Later, in 1998 Bollobás and Erdős [3] introduced general Randić index R_α, where α ia a real number, as

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

In order to attack some conjectures concerning the Randić index, Dvořák et al. introduced in [6] a variation of this index, denoted by R'. The variation of

[1]corresponding author (pavlovic@kg.ac.rs)

the Randić index of a graph G is given by

$$R'(G) = \sum_{uv \in E(G)} \frac{1}{\max\{d(u)d(v)\}}.$$

Although no application of the R' index in chemistry is known so far, nevertheless this index turns out to be very useful, especially from a mathematical point of view, since it is much easier to follow during graph modifications than the Randić index. Using the R' index, Cygan et al. [4] resolved the conjecture $R(G) \geq \mathrm{rad}(G) - 1$ given by Fajtlowicz 1988 in [7] for the case when G is a chemical graph. In [1] Andova et al. determined graphs with minimal and maximal value for the R' index , as well as graphs with minimal and maximal value of the R' index among trees and unicyclic graphs. They also showed that if G is a triangle free graph on n vertices with minimum degree $\delta(G)$, then $R'(G) \geq \delta$.

Now we define terms and symbols used in the paper. Let $G(k, n)$ be the set of connected simple n-vertex graphs with minimum vertex degree k. If u is a vertex of G, then $d(u)$ denotes the degree of the vertex u, that is, the number of edges of which u is an endpoint. Let $V(G)$, $E(G)$, $\delta(G)$ and $\Delta(G)$ denote the vertex set, edge set, minimum degree, and maximum degree of G, respectively. The complete split graph $K^*_{k,n-k}$ arises from the complete bipartite graph $K_{k,n-k}$ by adding edges to make the vertices in the partite set of size k pairwise adjacent. Let $\mathcal{G}_{n,p,k}$ be the family of complements of graphs consisting of an $(n-k-1)$-regular graph on p vertices together with $n-p$ isolated vertices. We also can describe $\mathcal{G}_{n,p,k}$ as the family of n-vertex graphs obtained from K_n by deleting the edges of an $(n-k-1)$-regular graph on p vertices.

In this paper we further investigate properties of the R' index with regard to minimum degree k. We found in $G(k, n)$ graphs for which the variation of the Randić index attains its minimum value. When $k \leq \frac{n}{2}$ the extremal graphs are complete split graphs $K^*_{k,n-k}$. For $k \geq \frac{n}{2}$ the extremal graphs belong to the family $\mathcal{G}_{n,\frac{n}{2},k}$. We proved next Theorem which match conjecture given by Aouchiche and Hansen about the Randić index in [2].

Theorem 1. If G is a graph of order n with $\delta(G) \geq k$, then

$$R'(G) \geq \begin{cases} \frac{n}{2} - \frac{1}{2}(\frac{1}{k} - \frac{1}{n-1})k(n-k) & \text{if } k \leq \frac{n}{2}, \\ \frac{n}{2} - \frac{1}{2}(\frac{1}{k} - \frac{1}{n-1})\frac{n^2}{4} & \text{if } \frac{n}{2} \leq k \leq n-2, \end{cases}$$

For $k \leq \frac{n}{2}$ equality holds if and only if $G = K^*_{k,n-k}$. For $k \geq \frac{n}{2}$ equality holds if $n \equiv 0 (\mathrm{mod}\ 4)$, or if $n \equiv 2 (\mathrm{mod}\ 4)$ and k is odd, and $G \in \mathcal{G}_{n,n/2,k}$.

The proof is based on the approach first time introduced in [12].

2. A QUADRATIC PROGRAMMING MODEL OF THE PROBLEM

First, we will give some linear equalities and nonlinear inequalities which must be satisfied in any graph from the class $G(k, n)$. Let $x_{i,j}$ denote the number of edges joining vertices of degrees i and j and n_i denote the number of vertices of degree n_i. The mathematical description of the problem P to determine minimum of $R'(G) = \sum_{k\le i\le j\le n-1} \frac{x_{i,j}}{\max\{ij\}} = \sum_{k\le i\le j\le n-1} \frac{x_{i,j}}{j}$ is:

$$\min \sum_{k\le i\le j\le n-1} \frac{x_{i,j}}{j}$$

subject to:

$$\begin{array}{l} 2x_{k,k} + x_{k,k+1} + x_{k,k+2} + \cdots + x_{k,n-1} = kn_k, \\ x_{k,k+1} + 2x_{k+1,k+1} + x_{k+1,k+2} + \cdots + x_{k+1,n-1} = (k+1)n_{k+1}, \\ \cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots \\ x_{k,n-1} + x_{k+1,n-1} + x_{k+2,n-1} + \cdots + 2x_{n-1,n-1} = (n-1)n_{n-1}, \end{array} \quad (1)$$

$$n_k + n_{k+1} + n_{k+2} + \cdots + n_{n-1} = n, \quad (2)$$

$$x_{i,j} \le n_i n_j, \qquad \text{for} \quad k \le i \le n-1, \quad i < j \le n-1, \quad (3)$$

$$x_{i,i} \le \binom{n_i}{2}, \qquad \text{for} \quad k \le i \le n-1, \quad (4)$$

$$x_{i,j},\ n_i \quad \text{are non-negative integers, for} \quad k \le i \le j \le n-1. \quad (5)$$

$(1-5)$ define a nonlinearly constrained optimization problem.

As it was done in [5], we divide the first equality from (1) by k, second by $k+1$, third by $k+2$ and so on, the last by $n-1$ and sum them all, and get

$$\sum_{k\le i\le j\le n-1} \left(\frac{1}{i} + \frac{1}{j}\right) x_{i,j} = n_k + n_{k+1} + n_{k+2} + \cdots + n_{n-1} = n,$$

because of (2). On the other side, $\frac{1}{j} = \frac{1}{2}(\frac{1}{i} + \frac{1}{j}) - \frac{1}{2}(\frac{1}{i} - \frac{1}{j})$. Then

$$\begin{aligned} R'(G) &= \sum_{k\le i\le j\le n-1} \frac{x_{i,j}}{j} = \frac{1}{2} \sum_{k\le i\le j\le n-1} \left(\frac{1}{i} + \frac{1}{j} - \left(\frac{1}{i} - \frac{1}{j}\right)\right) x_{i,j} \\ &= \frac{1}{2} \sum_{k\le i\le j\le n-1} \left(\frac{1}{i} + \frac{1}{j}\right) x_{i,j} - \frac{1}{2} \sum_{k\le i\le j\le n-1} \left(\frac{1}{i} - \frac{1}{j}\right) x_{i,j} \\ &= \frac{n}{2} - \frac{1}{2} \sum_{k\le i\le j\le n-1} \left(\frac{1}{i} - \frac{1}{j}\right) x_{i,j}. \end{aligned}$$

We will henceforth use the next expression (6) for the variation of the Randić index:

$$R'(G) = \frac{n}{2} - \frac{1}{2} \sum_{k\le i\le j\le n-1} \left(\frac{1}{i} - \frac{1}{j}\right) x_{i,j}. \quad (6)$$

Define the function

$$\gamma = \sum_{k\le i\le j\le n-1} \left(\frac{1}{i} - \frac{1}{j}\right) x_{i,j}. \quad (7)$$

Henceforth we will consider the problem of maximizing γ instead of minimizing $R'(G)$.

3. PROOF OF THE FIRST PART OF THEOREM 1 ($k \leq \frac{n}{2}$)

PROOF: Since the minimum degree is k, it is evident that $n_{n-1} \leq k$. Let m be the index such that $n_m + n_{m+1} + ... + n_{n-2} + n_{n-1} \geq k$ and $n_{m+1} + ... + n_{n-2} + n_{n-1} < k$. We distinguish two subcases: (a) for such m $n_m + ... + n_{n-2} + n_{n-1} = k$, and (b) $n_m + ... + n_{n-2} + n_{n-1} > k$.

Subcase a. $n_m + ... + n_{n-2} + n_{n-1} = k$. We have:

$$\begin{aligned}
\gamma &= \sum_{k \leq i < j \leq n-1} \left(\frac{1}{i} - \frac{1}{j}\right) x_{i,j} = \sum_{j=k+1}^{n-1} \left(\frac{1}{k} - \frac{1}{j}\right) x_{k,j} \\
&+ \sum_{j=k+2}^{n-1} \left(\frac{1}{k+1} - \frac{1}{j}\right) x_{k+1,j} + \sum_{j=k+3}^{n-1} \left(\frac{1}{k+2} - \frac{1}{j}\right) x_{k+2,j} \\
&+ \cdots + \sum_{j=m}^{n-1} \left(\frac{1}{m-1} - \frac{1}{j}\right) x_{m-1,j} + \sum_{m \leq i < j \leq n-1} \left(\frac{1}{i} - \frac{1}{j}\right) x_{i,j}.
\end{aligned}$$

$\sum_{j=i+1}^{n-1} (\frac{1}{i} - \frac{1}{j}) x_{i,j}$ represents weights of all edges which join vertices of degree i, with vertices of degree j, $i+1 \leq j \leq n-1$. We give the maximum possible weights to these edges. Since $n_m + n_{m+1} + \cdots + n_{n-1} = k$ and $\sum_{j=i+1}^{n-1} x_{i,j} \leq i n_i$, first we join a vertex of degree i to all k vertices of degrees $n-1, \ldots, m$ (maximum weights) and with $i-k$ vertices of other degrees j, $i+1 \leq j \leq m-1$. We will maximize the weights of these last $i-k$ edges joining a vertex of degree i to $i-k$ vertices of degree $m-1$. Thus,

$$\sum_{j=i+1}^{n-1} (\frac{1}{i} - \frac{1}{j}) x_{i,j} \leq n_i \left(\sum_{j=m}^{n-1} \left(\frac{1}{i} - \frac{1}{j}\right) n_j + \left(\frac{1}{i} - \frac{1}{m-1}\right)(i-k) \right).$$

Then

$$\begin{aligned}
\gamma &\leq \sum_{k \leq i \leq m-1} g(i) n_i + \sum_{m \leq i < j \leq n-1} \left(\frac{1}{i} - \frac{1}{j}\right) x_{i,j} \\
&= \Sigma_1 + \Sigma_2.
\end{aligned}$$

where $g(i) = \sum_{j=m}^{n-1} (\frac{1}{i} - \frac{1}{j}) n_j + (\frac{1}{i} - \frac{1}{m-1})(i-k)$. Since $f(x) = x(\frac{1}{x} - \frac{1}{y})$, for $0 < x < y$, is a decreasing function, we have for $k+1 \leq i \leq m-1$, $m \leq j \leq n-1$:

$$i(\frac{1}{i} - \frac{1}{j}) \leq k(\frac{1}{k} - \frac{1}{j}).$$

Therefore

$$g(i) \leq \frac{k}{i} \left(\sum_{j=m}^{n-1} (\frac{1}{k} - \frac{1}{j}) n_j + (\frac{1}{k} - \frac{1}{m-1})(i-k) \right)$$

$$
\begin{aligned}
&= (1-\frac{i-k}{i})\left(\sum_{j=m}^{n-1}(\frac{1}{k}-\frac{1}{j})n_j\right)+\frac{k(i-k)}{i}(\frac{1}{k}-\frac{1}{m-1})\\
&= \sum_{j=m}^{n-1}(\frac{1}{k}-\frac{1}{j})n_j+\frac{i-k}{i}\left((\frac{1}{k}-\frac{1}{m-1})k-\sum_{j=m}^{n-1}(\frac{1}{k}-\frac{1}{j})n_j\right)\\
&\le \sum_{j=m}^{n-1}(\frac{1}{k}-\frac{1}{j})n_j,
\end{aligned}
$$

because $\sum_{j=m}^{n-1} n_j = k$ and $m \le j \le n-1$. Since $n_k + \ldots + n_{m-1} = n-k$, we have

$$
\begin{aligned}
\Sigma_1 &= \sum_{k\le i\le m-1} g(i)n_i \le \left(\sum_{j=m}^{n-1}(\frac{1}{k}-\frac{1}{j})n_j\right)\sum_{i=k}^{m-1} n_i = (n-k)\sum_{j=m}^{n-1}(\frac{1}{k}-\frac{1}{j})n_j\\
&= \sum_{j=m}^{n-1}\left(\frac{1}{k}-\frac{1}{n-1}\right)(n-k)n_j-\sum_{j=m}^{n-2}\left(\frac{1}{k}-\frac{1}{n-1}\right)(n-k)n_j\\
&+ \sum_{j=m}^{n-2}\left(\frac{1}{k}-\frac{1}{j}\right)(n-k)n_j=\left(\frac{1}{k}-\frac{1}{n-1}\right)(n-k)k\\
&+ \sum_{j=m}^{n-2}\left(\left(\frac{1}{k}-\frac{1}{j}\right)-\left(\frac{1}{k}-\frac{1}{n-1}\right)\right)(n-k)n_j\\
&= \left(\frac{1}{k}-\frac{1}{n-1}\right)(n-k)k-\sum_{j=m}^{n-2}\left(\frac{1}{j}-\frac{1}{n-1}\right)(n-k)n_j.
\end{aligned}
$$

Since $x_{i,j} \le n_i n_j$, $m \le i < j \le n-1$, and $n_{n-1} = k - \sum_{j=m}^{n-2} n_j$, we have:

$$
\begin{aligned}
\Sigma_2 &= \sum_{m\le i<j\le n-1}\left(\frac{1}{i}-\frac{1}{j}\right)x_{i,j} \le \sum_{m\le i<j\le n-1}\left(\frac{1}{i}-\frac{1}{j}\right)n_in_j\\
&= \sum_{i=m}^{n-2}\left(\frac{1}{i}-\frac{1}{n-1}\right)n_i\left(k-\sum_{j=m}^{n-2}n_j\right)+\sum_{m\le i<j\le n-2}\left(\frac{1}{i}-\frac{1}{j}\right)n_in_j\\
&= k\sum_{i=m}^{n-2}\left(\frac{1}{i}-\frac{1}{n-1}\right)n_i-\sum_{i=m}^{n-2}\left(\frac{1}{i}-\frac{1}{n-1}\right)n_i^2\\
&+ \sum_{m\le i<j\le n-2}\left((\frac{1}{i}-\frac{1}{j})-(\frac{1}{i}-\frac{1}{n-1})-(\frac{1}{j}-\frac{1}{n-1})\right)n_in_j\\
&= k\sum_{i=m}^{n-2}\left(\frac{1}{i}-\frac{1}{n-1}\right)n_i-\sum_{i=m}^{n-2}\left(\frac{1}{i}-\frac{1}{n-1}\right)n_i^2\\
&- 2\sum_{m\le i<j\le n-2}\left(\frac{1}{j}-\frac{1}{n-1}\right)n_in_j
\end{aligned}
$$

Thus,

$$
\begin{aligned}
\gamma &\leq \Sigma_1 + \Sigma_2 \leq \left(\frac{1}{k} - \frac{1}{n-1}\right)(n-k)k \\
&- \sum_{i=m}^{n-2}\left(\frac{1}{i} - \frac{1}{n-1}\right)(n-k)n_i \\
&+ k\sum_{i=m}^{n-2}\left(\frac{1}{i} - \frac{1}{n-1}\right)n_i - \sum_{i=m}^{n-2}\left(\frac{1}{i} - \frac{1}{n-1}\right)n_i^2 \\
&- 2\sum_{m\leq i<j\leq n-2}\left(\frac{1}{j} - \frac{1}{n-1}\right)n_in_j = \left(\frac{1}{k} - \frac{1}{n-1}\right)(n-k)k \\
&- \sum_{i=m}^{n-2}\left(\frac{1}{i} - \frac{1}{n-1}\right)(n-2k)n_i - \sum_{i=m}^{n-2}\left(\frac{1}{i} - \frac{1}{n-1}\right)n_i^2 \\
&- 2\sum_{m\leq i<j\leq n-2}\left(\frac{1}{j} - \frac{1}{n-1}\right)n_in_j \leq \left(\frac{1}{k} - \frac{1}{n-1}\right)(n-k)k.
\end{aligned}
$$

The last inequality follows because $k \leq \frac{n}{2}$. Equality holds when $n_i = 0$ for $k+1 \leq i \leq n-2$, $n_k = n-k$, $n_{n-1} = k$, $x_{k,n-1} = (n-k)k$, $x_{n-1,n-1} = \binom{k}{2}$, and all other $x_{i,j}$ are equal to zero. Thus, graphs for which variation of the Randić index attains its minimum value are $K^*_{k,n-k}$.

Subcase b. We put $n_m = n_{m'} + n_{m''}$, such that $n_{m''} + n_{m+1} + ... + n_{n-1} = k$. Then $n_k + \cdots + n_{m-1} + n_{m'} = n-k$. We will color the vertices of degree m with red and white, such that the number of red vertices is $n_{m''}$. Denote by $x_{i,m'}(x_{i,m''})$ for $i \neq m$, the number of edges between vertices of degree i and the white (red) vertices of degree m, by $x_{m',m'}$ $(x_{m'',m''})$ the number of edges between white (red) vertices of degree m, and by $x_{m',m''}$ the number of edges between white and red vertices of degree m. Then $x_{i,m} = x_{i,m'} + x_{i,m''}$ for $i \neq m$, and $x_{m,m} = x_{m',m'} + x_{m',m''} + x_{m'',m''}$. We will replace system (1) by:

$$
\begin{aligned}
x_{k,i} + \cdots + x_{i,m-1} + x_{i,m'} + x_{i,m''} + x_{i,m+1} + \cdots + x_{i,n-1} &= in_i, \\
k \leq i \leq n-1, i \neq m&, \\
x_{k,m'} + \cdots + x_{m-1,m'} + 2x_{m',m'} + x_{m',m''} + x_{m',m+1} + \cdots + x_{m',n-1} &= mn_{m'}, \\
x_{k,m''} + \cdots + x_{m-1,m''} + x_{m',m''} + 2x_{m'',m''} + x_{m'',m+1} + \cdots + x_{m'',n-1} &= mn_{m''},
\end{aligned}
\qquad (\tilde{1})
$$

We will proceed similarly as in the subcase a. The rest of the proof is omitted, because it is similar to the one of subcase a. □

4. PROOF OF THE SECOND PART OF THEOREM 1 ($k \geq \frac{n}{2}$)

We put:

$$x_{i,j} = n_i n_j - y_{i,j} \qquad \text{for} \qquad k \le i \le n-1,\ i < j \le n-1,$$
$$x_{i,i} = \binom{n_i}{2} - y_{i,i} \qquad \text{for} \qquad k \le i \le n-1. \tag{8}$$

A vertex of degree $n-1$ is adjacent to all other vertices. Thus $y_{i,n-1} = 0$ for $k \le i \le n-1$ and $n_{n-1} \le k$, or the minimum degree would be greater than k. After substitution of $x_{i,j}$ and $x_{i,i}$ from (8) into the function γ and (1), we rewrite the optimization problem using the same objective function (call the rewritten problem $\overline{P}$) as:

$$\max \sum_{k\le i<j\le n-1} \left(\frac{1}{i} - \frac{1}{j}\right) n_i n_j - \sum_{k\le i<j\le n-2} \left(\frac{1}{i} - \frac{1}{j}\right) y_{i,j}$$

subject to

$$\begin{array}{l} 2y_{k,k} + y_{k,k+1} + y_{k,k+2} + \cdots + y_{k,n-2} = (n-k-1)n_k, \\ y_{k,k+1} + 2y_{k+1,k+1} + y_{k+1,k+2} + \cdots + y_{k+1,n-2} = (n-k-2)n_{k+1}, \\ \cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots \\ y_{k,n-2} + y_{k+1,n-2} + y_{k+2,n-2} + \cdots + 2y_{n-2,n-2} = n_{n-2}, \end{array} \tag{1'}$$

$$n_k + n_{k+1} + n_{k+2} + \cdots + n_{n-1} = n, \tag{2}$$

$$n_i \ge 0, \qquad \text{for} \quad k \le i \le n-1, \tag{9}$$
$$y_{i,j} \ge 0, \qquad \text{for} \quad k \le i \le n-2,\ i \le j \le n-2, \tag{10}$$
$$n_{n-1} \le k, \tag{11}$$

$$y_{i,j},\ n_i \quad \text{are integers for} \quad k \le i \le j \le n-1. \tag{5'}$$

We obtained equalities (1′) from the corresponding equalities (1). Let $(n_k, n_{k+1}, \ldots, n_{n-1}, y_{k,k}, y_{k,k+1}, \ldots, y_{n-2,n-2})$ be a feasible point for $\overline{P}$; we use Ω or (N, Y) to denote this point. Let $\gamma_1 = \sum_{k\le i<j\le n-1}(\frac{1}{i}-\frac{1}{j})n_i n_j$ and $\gamma_2 = -\sum_{k\le i<j\le n-2}(\frac{1}{i}-\frac{1}{j})y_{i,j}$. Now $\max\gamma \le \max\gamma_1 + \max\gamma_2$, where the maxima are subject to (1′), (2), (9–11), (5′). It is evident that $\max\gamma_2 = 0$, and it is achieved by setting $y_{i,j} = 0$ for $k \le i \le n-2$ and $i < j \le n-2$ and setting $y_{i,i} = \frac{(n-i-1)n_i}{2}$ for $k \le i \le n-2$. The variables n_i must satisfy (2), (9), (11) and (5′). Hence, there are many extreme points for γ_2. Let us denote by $(n^*_k, n^*_{k+1}, \ldots, n^*_{n-1})$ or N^* the optimal point for γ_1. Let $Y^* = (y^*_{k,k}, y^*_{k,k+1}, \ldots, y^*_{n-2,n-2})$, where $y^*_{i,j} = 0$ for $i \ne j$ and $y^*_{i,i} = \frac{(n-i-1)n^*_i}{2}$. Note that Y^* is the optimal point for γ_2 if $y^*_{i,j}$ are integers, and (N^*, Y^*) will be the optimal point for γ. In order to find N^* we can neglect constraints (1′) and (10), because for γ_1 only constraints (2), (9) and (11) are relevant. We omit constraint (11), because it is not necessary and would complicate the calculation. We also neglect constraint (5′), but we will keep it in mind.

We will need the following theorems.

Theorem 1.4.10 from [15]. A two times differentiable function f on open convex set C is concave if and only if Hessian matrix

$$H(x) = \left[\frac{\partial^2 f(x)}{\partial x_i \partial x_j}\right]$$

is negative-semidefinite matrix for $\forall x \in C$.

Generalized Sylvester's cryterion. A $n \times n$ Hermitian matrix $A = (a_{i,j})$ is negative-definite if and only if members of the sequence $1, D_1, D_2, \ldots, D_n$ change the sign, where D_i are the principal minors, that is $(D_1 < 0, D_2 > 0, \ldots)$.

From (2), we have $n_{n-1} = n - \sum_{j=k}^{n-2} n_j$. We rewrite γ_1:

$$\begin{aligned}
\gamma_1 &= \sum_{k\le i<j\le n-2} \left(\frac{1}{i} - \frac{1}{j}\right) n_i n_j + \sum_{i=k}^{n-2} \left(\frac{1}{i} - \frac{1}{n-1}\right) n_i (n - \sum_{j=k}^{n-2} n_j) \\
&= n \sum_{i=k}^{n-2} \left(\frac{1}{i} - \frac{1}{n-1}\right) n_i - \sum_{i=k}^{n-2} \left(\frac{1}{i} - \frac{1}{n-1}\right) n_i^2 \\
&+ \sum_{k\le i<j\le n-2} \left((\frac{1}{i} - \frac{1}{j}) - (\frac{1}{i} - \frac{1}{n-1}) - (\frac{1}{j} - \frac{1}{n-1}) \right) n_i n_j \\
&= n \sum_{i=k}^{n-2} \left(\frac{1}{i} - \frac{1}{n-1}\right) n_i - \sum_{i=k}^{n-2} \left(\frac{1}{i} - \frac{1}{n-1}\right) n_i^2 \\
&- 2 \sum_{k\le i<j\le n-2} \left(\frac{1}{j} - \frac{1}{n-1}\right) n_i n_j \qquad (12)
\end{aligned}$$

Define a function $\bar{\gamma}_1$ by $\bar{\gamma}_1(n_k, ..., n_{n-2}) = n \sum_{i=k}^{n-2} \left(\frac{1}{i} - \frac{1}{n-1}\right) n_i - \sum_{i=k}^{n-2} \left(\frac{1}{i} - \frac{1}{n-1}\right) n_i^2 - 2 \sum_{k\le i<j\le n-2} \left(\frac{1}{j} - \frac{1}{n-1}\right) n_i n_j$ (see (12)). Let $X = \{(n_k, ..., n_{n-1}) \mid n_k + ... + n_{n-1} = n\}$. Note that $\gamma_1(n_k, ..., n_{n-1}) = \bar{\gamma}_1(n_k, ..., n_{n-2})$ for $(n_k, ..., n_{n-1}) \in X$. We will study $\bar{\gamma}_1$ on $\mathbb{R}^{n-k-1}$ instead of γ_1 on X. The point $(n_k, ..., n_{n-2}) \in \mathbb{R}^{n-k-1}$ corresponds to $(n_k, ..., n_{n-2}, n - \sum_{j=k}^{n-2} n_j) \in \mathbb{R}^{n-k}$ on the set X. Let us notice that $\bar{\gamma}_1$ on $\mathbb{R}^{n-k-1}$ is concave function. The j-th principal minor is

$$D_j = (-2)^j \begin{vmatrix}
(\frac{1}{k} - \frac{1}{n-1}) & (\frac{1}{k+1} - \frac{1}{n-1}) & (\frac{1}{k+2} - \frac{1}{n-1}) & \cdots & (\frac{1}{k+j-1} - \frac{1}{n-1}) \\
(\frac{1}{k+1} - \frac{1}{n-1}) & (\frac{1}{k+1} - \frac{1}{n-1}) & (\frac{1}{k+2} - \frac{1}{n-1}) & \cdots & (\frac{1}{k+j-1} - \frac{1}{n-1}) \\
(\frac{1}{k+2} - \frac{1}{n-1}) & (\frac{1}{k+2} - \frac{1}{n-1}) & (\frac{1}{k+2} - \frac{1}{n-1}) & \cdots & (\frac{1}{k+j-1} - \frac{1}{n-1}) \\
\vdots & \vdots & \vdots & \ddots & \vdots \\
(\frac{1}{k+j-1} - \frac{1}{n-1}) & (\frac{1}{k+j-1} - \frac{1}{n-1}) & (\frac{1}{k+j-1} - \frac{1}{n-1}) & \cdots & (\frac{1}{k+j-1} - \frac{1}{n-1})
\end{vmatrix}.$$

It is not difficult to find that $D_j = 2^j(-1)^j(\frac{1}{k} - \frac{1}{k+1})(\frac{1}{k+1} - \frac{1}{k+2})(\frac{1}{k+2} - \frac{1}{k+3}) \cdots (\frac{1}{k+j-2} - \frac{1}{k+j-1})(\frac{1}{k+j-1} - \frac{1}{n-1})$. Using Sylvester's cryterion we conclude that $\bar{\gamma}_1$ is concave function.

We consider the problem $\overline{P^1}$ of maximizing $\bar{\gamma}_1$:

$$\max\ n \sum_{i=k}^{n-2} \left(\frac{1}{i} - \frac{1}{n-1}\right) n_i - \sum_{i=k}^{n-2} \left(\frac{1}{i} - \frac{1}{n-1}\right) n_i^2 - 2 \sum_{k\le i<j\le n-2} \left(\frac{1}{j} - \frac{1}{n-1}\right) n_i n_j$$

subject to

$$n_i \ge 0 \quad \text{for} \quad k \le i \le n-2, \qquad (9)$$

instead of the problem: $\max \gamma_1$ subject to (2) and (9). Let N denote a feasible point $(n_k, \ldots, n_{n-2})$ for problem $\overline{P^1}$. We will show that N_1^* is an optimal point for the problem $\overline{P^1}$, where N_1^* is defined by $n_k = \frac{n}{2}, n_i = 0$ for $k+1 \le i \le n-2$.

Lemma 1. *The function γ_1, subject to (2) and (9), attains its maximum value γ_1^* equal to $\frac{n^2}{4}(\frac{1}{k} - \frac{1}{n-1})$ at the point $(\frac{n}{2}, 0, 0, \ldots, 0, \frac{n}{2}) \in \mathbb{R}^{n-k}$.*

PROOF: We distinguish two subcases: (1a) $\Delta(G) = n-1$, and (1b) $\Delta(G) < n-1$.

Subcase 1a. We will find point $N = (n_k, ..., n_{n-2})$ for which $\partial \bar{\gamma}_1 / \partial n_i = 0$, $k \le i \le n-2$, respectively:

$$n\left(\frac{1}{k} - \frac{1}{n-1}\right) - 2\left(\frac{1}{k} - \frac{1}{n-1}\right)n_k - 2\sum_{k<j\le n-2}\left(\frac{1}{j} - \frac{1}{n-1}\right)n_j = 0, \qquad (13)$$

$$\begin{aligned} & n\left(\frac{1}{i} - \frac{1}{n-1}\right) - 2\left(\frac{1}{i} - \frac{1}{n-1}\right)n_i - 2\sum_{k\le j<i}\left(\frac{1}{i} - \frac{1}{n-1}\right)n_j \\ - \; & 2\sum_{i<j\le n-2}\left(\frac{1}{j} - \frac{1}{n-1}\right)n_j = 0, \qquad \text{for } \; k+1 \le i \le n-2, \qquad (14) \end{aligned}$$

It is easy to see that the point $(\frac{n}{2}, 0, 0, \ldots, 0)$ satisfies equalities conditions $(13-14)$. Since $\bar{\gamma}_1$ is a concave function the point $(\frac{n}{2}, 0, 0, \ldots, 0)$ is a maximum point and the maximum value $\bar{\gamma}_1^* = \gamma_1^*$ is

$$\frac{n^2}{4}(\frac{1}{k} - \frac{1}{n-1}).$$

To point $N_1^* = (\frac{n}{2}, 0, 0, \ldots, 0) \in \mathbb{R}^{n-k-1}$ corresponds point $N^* = (\frac{n}{2}, 0, 0, \ldots, 0, \frac{n}{2}) \in \mathbb{R}^{n-k}$.

Subcase 1b. Let $m = \Delta(G)$. For this case the proof is similar to that of subcase 1a and is omitted. The maximum value of γ_1 is

$$\gamma_1^m = \left(\frac{1}{k} - \frac{1}{m}\right)\frac{n^2}{4}.$$

This value is attained at the point $n_k = \frac{n}{2}, n_i = 0$ for $k+1 \le i \le m-1$, and $n_m = \frac{n}{2}$. Since $\gamma_1^* > \gamma_1^m$ for this case, we conclude that γ_1^* is the maximum value, attained at N^* on the set of all feasible points. □

We have proved that γ_1 attains its maximum at N^*. Now observe that γ_2 attains its maximum value, which is 0, at the point Y_1^* defined by setting $y_{k,k} = \frac{(n-k-1)n}{4}$ and all other $y_{i,j} = 0$. We conclude that the variation of the Randić index attains its minimum on graphs for which $n_k = n_{n-1} = n/2, x_{k,k} = n(2k -$

$n)/8, x_{k,n-1} = n^2/4, x_{n-1,n-1} = n(n-2)/8$, and all other $x_{i,j}, x_{i,i}$ and n_i are equal to zero. These values are integers only if $n \equiv 0 (\text{mod } 4)$, or if $n \equiv 2 (\text{mod } 4)$ and k is odd, and these graphs lie in $\mathcal{G}_{n,n/2,k}$.

Thus, we come to our conclusion:

The second part of Theorem 1. *If $G \in G(k,n)$, then*

$$R'(G) \geq \frac{n}{2} - \frac{n^2}{8}\left(\frac{1}{k} - \frac{1}{n-1}\right).$$

If $n \equiv 0 (\text{mod } 4)$, or if $n \equiv 2 (\text{mod } 4)$ and k is odd, this value is attained by graphs $G \in \mathcal{G}_{n,n/2,k}$ for which $n_k = n_{n-1} = n/2, x_{k,k} = n(2k-n)/8, x_{k,n-1} = n^2/4, x_{n-1,n-1} = n(n-2)/8$, and all other $x_{i,j}, x_{i,i}$ and n_i are equal to zero.

Furthermore, if $G \in \mathcal{G}_{n,p,k}$, then $R'(G) = \frac{n}{2} - \frac{1}{2}(\frac{1}{k} - \frac{1}{n-1})p(n-p)$. Now we give conjecture about extremal graphs for the other parity of n and k.

Conjecture. If $G \in G(k,n)$ and if

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

then

$$R'(G) \geq \frac{n}{2} - \frac{1}{2}(\frac{1}{k} - \frac{1}{n-1})p(n-p) \qquad \text{if } \frac{n}{2} < k \leq n-2,$$

where p and n are given above. Equality holds if and only if $G \in \mathcal{G}_{n,p,k}$.

The proof of this conjecture is more complicated than for the case $n \equiv 0 (\text{mod } 4)$, or if $n \equiv 2 (\text{mod } 4)$ and k is odd and we leave it as an open problem. More information on γ_1 function could be obtained using maximizing technique given in [14] or approach in [11].

Let $G(k,m,n)$ be the set of connected simple n-vertex graphs with minimum vertex degree k and maximum vertex degree m, where $k \leq m \leq n-2$. Let $\mathcal{G}_{n,p,k,m}$ be the family of complements of graphs consisting of an $(n-k-1)$-regular graph on p vertices and $(n-m-1)$-regular graph on $n-p$ vertices. Since the proof of the next theorem is similar to those of Theorems 1, we omit them and just write down the theorem.

Theorem 2. *If G is a graph of order n with $\delta(G) \geq k$ and $\triangle(G) \leq m$, then*

$$R'(G) \geq \begin{cases} \frac{n}{2} - \frac{1}{2}(\frac{1}{k} - \frac{1}{m})k(n-k) & \text{if } k \leq \frac{n}{2}, \quad \text{and } n-k \leq m \leq n-2 \\ \frac{n}{2} - \frac{1}{2}(\frac{1}{k} - \frac{1}{m})\frac{n^2}{4} & \text{if } \frac{n}{2} \leq k \leq m \leq n-2, \end{cases}$$

For $k \leq \frac{n}{2}$, equality holds if k is even, or k and $n-m$ are odd, and this value is attained by graphs for which $n_k = n-k, n_m = k, x_{k,m} = (n-k)k, x_{m,m} =$

$k(k+m-n)/2$, and all other $x_{i,j}, x_{i,i}$ and n_i are equal to zero. For $k \geq \frac{n}{2}$ equality holds if $n \equiv 0 (\text{mod } 4)$, or if $n \equiv 2 (\text{mod } 4)$, and k and m are odd, and this value is attained by graphs $G \in \mathcal{G}_{n,n/2,k,m}$ for which $n_k = n_m = n/2, x_{k,k} = n(2k-n)/8, x_{k,m} = n^2/4, x_{m,m} = n(2m-n)/8$, and all other $x_{i,j}, x_{i,i}$ and n_i are equal to zero.

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References

[1] V. Andova, M. Knor, P. Potočnik, R. Škrekovski, *On a variation of the Randić index*, Australian Journal of Combinatorics, 56 (2013), 61-67.

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

[3] B. Bollobás, P. Erdős, *Graphs of Extremal Weights*, Ars Combinatoria, 50 (1998), 225 - 233.

[4] M. Cygan, M. Pilipczuk, R. Škrekovski, *On the inequality between radius and Randić index for Graphs*, MATCH - Commun. Math. Comput. Chem., 67 (2012), 451-466.

[5] T. Divnić, Lj. Pavlović, *Proof of the first part of the conjecture of Aouchiche and Hansen about the Randić index*, Discrete Applied Mathematics, Vol.161, Issues 7-8,(2013), pp. 953-960.

[6] Dvořák, B. Lidicky, R. Škrekovski, *Randić index and the diameter of a graph*, European Journal of Combinatorics, 32 (2011),434-442.

[7] S. Fajtlowicz (1998), *Written on the Wall*, Conjectures derived on the basis of the program Galatea Gabriella Graffiti, University of Houston.

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

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

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

[11] B. Liu, Lj. Pavlović, J. Liu, T. Divnić, M. Stojanović, *On the conjecture of Aouchiche and Hansen about the Randić index*, Discrete Mathematics, Vol. 313, Issue 3 (2013), pp. 225-235.

[12] Lj. Pavlović, T. Divnić, *A quadratic programming approach to the Randić index*, European Journal of Operational Research, 2007, Vol. 176, Issue 1, pp. 435-444.

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

[14] I. Tomescu, R. Marinescu-Ghemeci, G. Mihai, *On dense graphs having minimum Randić index*, Romanian J. of Information Science and Technology (ROMJIST), Vol. 12, (4), 2009, pp. 455-465.
[15] V. Vujčić, M. Ašić, N. Miličić, *Matematičko programiranje*, Matematički Institut, Beograd (1980).