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The variation of the Randić index with regard to minimum and maximum degree

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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 $k \leq \frac{n}{2}$ 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 $k \geq \frac{n}{2}$ 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.

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 [15], 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 [15] 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 is 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 the Randić index of a graph G is given by

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

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Dvořák et al. [6] proved for every connected graph $R'(G) \geq d(G)$, where $d(G)$ is the diameter of G, which implies $R(G) \geq d(G)$. This index is very useful because it is much easier to calculate 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 in 1998 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 $R'(G) \geq \delta$. Liu in [11] gave an equivalent expression for this index. Using it, he showed in a different way, that if G is a triangle free graph with order n and the minimum degree $\delta \geq k$ $(k \leq \frac{n}{2})$, then $R'(G) \geq k$, where equality holds if and only if $G \cong K_{k,n-k}$. In [12] Liu characterized the extremal trees achieving the minimum value of R' among trees with given number of vertices and leaves. Further, he characterized the extremal graphs achieving the minimum value of R' for connected graphs with given number of vertices and girth.

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. 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 matches 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*

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

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 $n \equiv 0 \pmod 4$, or if $n \equiv 2 \pmod 4$ and k is odd, and $G \in \mathcal{G}_{n,n/2,k}$.

The proof is based on the approach first time introduced in [14].

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 i. The mathematical description of the problem P to determine minimum of $R'(G) = \sum_{k \leq i \leq j \leq n-1} \frac{x_{i,j}}{\max\{i,j\}} = \sum_{k \leq i \leq j \leq n-1} \frac{x_{i,j}}{j}$ is:

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

subject to:

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

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

$$x_{i,j} \leq n_i n_j, \quad \text{for } k \leq i \leq n-1,\ i < j \leq n-1, \tag{3}$$

$$x_{i,i} \leq \binom{n_i}{2}, \quad \text{for } k \leq i \leq n-1, \tag{4}$$

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

Constraints (1)–(5) define a nonlinearly 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

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

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