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Proof of the first part of the conjecture of Aouchiche and Hansen about the Randić index

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ABSTRACT

Let $G(k, n)$ be the set of connected simple n-vertex graphs with minimum vertex degree k. The Randić index $R(G)$ of a graph G is defined by: $R(G) = \sum_{uv\in E(G)} \frac{1}{\sqrt{d(u)d(v)}}$, where $d(u)$ is the degree of vertex u and the summation extends over all edges uv of G. In this paper we prove for $k \le \frac{n}{2}$ the conjecture of Aouchiche and Hansen about the graphs in $G(k, n)$ for which the Randić index attains its minimum value. We show that the extremal graphs are complete split graphs $K^*_{k,n-k}$, which have only 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. At the end we generalize our results to graphs with prescribed maximum degree q.

1. Introduction

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. 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 [22], 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. Randić himself demonstrated [22] that his 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; several books are devoted to it [11–13].

In [9] Fajtlowicz mentions that Bollobás and Erdős asked for the minimum value of the Randić index for the graphs in $G(k, n)$. This problem is difficult, and only a few partial results have been achieved. In [4] Bollobás and Erdős found the extremal graph when $k = 1$; it is a star. For $k = 2$ the problem is solved in [8]; the extremal graph is the complete split graph $K^*_{2,n-2}$. The 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. In these papers a graph-theoretical approach was used. In [21,16] the problem is solved for $k = 1$ and $k = 2$, respectively, using linear programming. In [17] Pavlović found the extremal graph for $k = \lfloor \frac{n}{2} \rfloor$ using a quadratic programming technique and considered the case $n_k \ge n - k$ [18,20], where n_k denotes the number of vertices of degree k. The system AutoGraphiX is helpful for finding extremal graphs [1–3,5,6] and for making conjectures about them. In [10] a lower bound was found for $R(G) - R(G - v)$, where v is a vertex of minimum degree $\delta(G)$ and $G - v$ denotes the graph obtained from G by deleting v and all its incident edges.

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Delorme, Favaron, and Rautenbach [8] posed the first conjecture about this problem. Aouchiche and Hansen [1] refuted this conjecture by using the system AutoGraphiX [7] and made a new more precise conjecture. Let

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

and let $\overline{G}_{n,p,k}$ be the complement of a graph $G_{n,p,k}$ consisting of an $(n-k-1)$-regular graph on p vertices together with $n-p$ isolated vertices.

Conjecture ([1]). *If G is a graph of order n with $\delta(G) \geq k$, 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 k_n and p are given above, with equality if and only if G is a complete split graph $K^*_{k,n-k}$ for $k < k_n$, and if and only if G is $\overline{G}_{n,p,k}$ for $k \geq k_n$.

Li, Liu and Liu [14] claimed that they had proved this conjecture completely, but Pavlović [19] showed that their proof is not correct from the beginning.

Since $\frac{k(k-1)}{2(n-1)} + \frac{k(n-k)}{\sqrt{k(n-1)}} = \frac{n}{2} - \frac{1}{2}(\frac{1}{\sqrt{k}} - \frac{1}{\sqrt{n-1}})^2 k(n-k)$, we will prove the part of this conjecture for $k \leq \frac{n}{2}$. For $k \geq \frac{n}{2}$ this conjecture is proven in other manuscript [15].

In this paper we prove Theorem 1. 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.

Theorem 1. *If $k \leq \frac{n}{2}$, and graph G belongs to the class $G(k, n)$, then*

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

This value is attained by graphs $G = K^*_{k,n-k}$ for which $n_k = n-k$, $n_{n-1} = k$, $x_{k,n-1} = (n-k)k$, $x_{n-1,n-1} = k(k-1)/2$, and all other $x_{i,j}$, $x_{i,i}$ and n_i are equal to zero.

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

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

subject to:

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

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

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

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

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

(1)–(5) define a nonlinearly constrained optimization problem.