Available online at www.sciencedirect.com
ScienceDirect
European Journal of Operational Research 180 (2007) 369–377
EUROPEAN JOURNAL OF OPERATIONAL RESEARCH
www.elsevier.com/locate/ejor

Decision Support

On the conjecture of Delorme, Favaron and Rautenbach about the Randić index

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Received 29 September 2004; accepted 27 February 2006
Available online 8 June 2006

Abstract

Let $G(k,n)$ be the set of connected graphs without multiple edges or loops which have n vertices and the minimum degree of vertices is k. The Randić index $\chi = \chi(G)$ of a graph G is defined by: $\chi = \sum_{(uv)} (\delta_u \delta_v)^{-1/2}$, where δ_u is the degree of vertex u and the summation extends over all edges (uv) of G. In this paper we prove the conjecture of Delorme, Favaron and Rautenbach about the graphs for which the Randić index attains its minimum value when $k = \lfloor \frac{n}{2} \rfloor$. We show that the extremal graphs must have $n - k$ vertices of degree k and k vertices of degree $n - 1$.

Keywords: Quadratic programming; Randić index; Kuhn–Tucker theorem

1. Introduction

Let $G(k,n)$ be the set of connected graphs without multiple edges or loops which have n vertices and the minimum degree of vertices is k. If u is a vertex of G, then δ_u denotes 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 $\chi = \chi(G)$ of a graph G defined in [17] is: $\chi = \sum_{(uv)} (\delta_u \delta_v)^{-1/2}$, where the summation extends over all edges (uv) of G. Randić himself demonstrated [17] that his index is well correlated with a variety of physico-chemical properties of alcanes. χ became one of the most popular molecular descriptors to which two books are devoted [10,12]. Initially the Randić connectivity index was studied only by chemists [10,11], but recently it attracted the attention also of mathematicians.

One of the mathematical questions asked in connection with χ is which graphs in a given class of graphs have maximum and minimum χ values [2]. In [6] Fajtlowitcz mentions that Bollobás and Erdős asked for

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0377-2217/$ - see front matter
doi:10.1016/j.ejor.2006.02.035

the minimum value on the Randić index for the graphs in $G(k,n)$. The solution of such problems turned out to be difficult, and only a few partial results have been achieved so far. In [2] Bollobás and Erdős found the extremal graph when $k=1$. It is a star. For $k=2$ the problem is solved in [9] and the extremal graph is a complete split graph, that is, it has to have $n_2 = n-2$ and $n_{n-1} = 2$. In these papers a graph theoretical approach has been used. In other papers [3–5,7,8] a linear programming and a quadratic programming technique [14] for finding extremal graphs has been used. In [15,16] the problem is solved for $k=1$ and $k=2$ respectively using linear programming. Delorme, Favaron and Rautenbach gave a conjecture about this problem [9]. The conjecture is that the Randić index for graphs in $G(k,n)$, where $1 \leqslant k \leqslant \frac{n}{2}$ attains its minimum value for the graph $K^*_{k,n-k}$ which arises from complete bipartite graph $K_{k,n-k}$ by joining all pairs of vertices in the partite set with k vertices by a new edge. In this paper we prove this conjecture when $k = n/2$ (n is an even number) or $k = (n-1)/2$ (n is an odd number). The more general ($1 \leqslant k \leqslant n-2$) and precise conjecture about the Randić index is given in [1].

2. A quadratic programming model of the problem

At first, we will give some linear equalities and nonlinear inequalities which must be satisfied in any above mentioned graph. Denote by $x_{i,j}$ ($x_{i,j} \geqslant 0$), the number of edges joining the vertices of degrees i and j. The mathematical description of the problem (P) is

$$\min \quad \chi = \sum_{\substack{k \leqslant i \leqslant n-1 \\ i \leqslant j \leqslant n-1}} \frac{x_{i,j}}{\sqrt{ij}}$$

subject to:

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

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

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

and

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

(A)–(D) define a nonlinearly constrained optimization problem. With regard to (A), Randić index is

$$\chi = \frac{n}{2} - \frac{1}{2} \sum_{\substack{k \leqslant i \leqslant n-1 \\ i \leqslant j \leqslant n-1}} \left(\frac{1}{\sqrt{i}} - \frac{1}{\sqrt{j}}\right)^2 x_{i,j} \tag{1}$$

and we will use further this expression for the Randić index.

3. Results

We will consider the case 1: $k = \frac{n}{2}$ for an even n and case 2: $k = \frac{n-1}{2}$ for an odd n.

Theorem 1. *Let $G(k,n)$ be a set of connected graphs without multiple edges or loops which have n vertices and the minimum degree of vertices is k. If $k = \lfloor \frac{n}{2} \rfloor$, then the minimum value of the Randić index for graphs in $G(k,n)$ is*