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On a conjecture of the Randić index and the minimum degree of graphs☆

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ABSTRACT

The Randić index $R(G)$ of a graph G is defined by $R(G) = \sum_{uv} \frac{1}{\sqrt{d(u)d(v)}}$, where $d(u)$ is the degree of a vertex u and the summation extends over all edges uv of G. Delorme et al. (2002) [6] put forward a conjecture concerning the minimum Randić index among all n-vertex connected graphs with the minimum degree at least k. In this work, we show that the conjecture is true given the graph contains k vertices of degree $n-1$. Further, it is true among k-trees.

1. Introduction

The Randić index $R = R(G)$ of a graph G is defined as follows:

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

where $d(u)$ denotes the degree of a vertex u and the summation runs over all edges uv of G. This topological index was first proposed by Randić [20] in 1975, suitable for measuring the extent of branching of the carbon-atom skeleton of saturated hydrocarbons. It is well correlated with a variety of physico-chemical properties of alkanes. And it is one of the most popular molecular descriptors to which four books [13–15,9] are devoted.

In this paper, we only consider finite, undirected and simple graphs. The *minimum degree* of a graph G, denoted by $\delta(G)$, is the minimum degree among its vertices. Harary and Palmer [12] defined an n-plex as an n-dimensional complex in which every k-simplex with $k < n$ is contained in an n-complex. For convenience 0-simplexes, 1-simplexes, and 2-simplexes are called points, lines, and cells respectively. The two-dimensional trees, also called 2-trees can now be defined inductively. The 2-plex with three points is a 2-tree and a 2-tree with $p+1$ points is obtained from a 2-tree with p points by adjoining a new point w adjoint to each of two adjacent points u and v together with the accompanying cell u, v, w. The definition of a k-tree for $k > 2$ is similar. We define a leaf as a vertex u of a k-tree with degree $d(u) = k$. Note that for any vertex u of a k-tree, $k \le d(u) \le n-1$. There are at least two leaves in any k-tree of order $n (k \le n-1)$. Note that a 1-tree is a tree in traditional graph theory. For undefined terminology and notations we refer the reader to the book of Bondy and Murty [3].

One of the mathematical questions asked in connection with R is to figure out which graphs among a given class of graphs have the maximum and minimum values of R. In [7] Fajtlowicz mentioned that Bollobás and Erdős asked for the minimum

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value of the Randić index among the connected n-vertex graphs with minimum degree k. 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 that for a connected n-vertex graph G:

$$R(G) \geq \sqrt{n-1},$$

the equality holds if and only if G is a star. Delorme, Favaron and Rautenbach [6] solved the problem for $k = 2$ and gave a stronger result, say, if the minimum degree is at least 2, then

$$R(G) \geq \frac{2n-4}{\sqrt{2n-2}} + \frac{1}{n-1},$$

the equality holds if and only if $G \cong K^{\star}_{2,n-2}$, which arises from complete bipartite graph $K_{2,n-2}$ by joining vertices in the partite set with 2 vertices by a new edge. Further, they proposed a conjecture concerning the minimum value of R among all connected n-vertex graphs with minimum degree at least k.

Conjecture 1.1. *For any connected n-vertex graph with minimum degree at least k, we have*

$$R(G) \geq \frac{k(n-k)}{\sqrt{k(n-1)}} + \frac{k(k-1)}{2(n-1)},$$

the equality holds if and only if $G \cong K^{\star}_{k,n-k}$, *which arises from complete bipartite graph* $K_{k,n-k}$ *by joining each pair of vertices in the partite set with k vertices by a new edge.*

In these papers a graph theoretical approach has been used. In other papers [4,5,8,10,11] a linear programming and a quadratic programming technique [18] for finding extremal graphs have been used.

In [16,19] the problem is solved for $k = 1$ and $k = 2$ respectively using linear programming. Using again linear programming, Pavlović [17] proved that Conjecture 1.1 holds when $k = (n-1)/2$ or $k = n/2$. Divnić and Pavlović [18] proved that Conjecture 1.1 holds when $k \leq n/2$ and $n_k \geq n-k$, where n_i denotes the number of vertices of degree i. Li and Shi (see [9]) showed that the conjecture holds when $k = 3$ and it is true for all chemical graphs. Further, they proved that it is true when $n \geq 3k^3/2$ and $k \geq 4$. Although many evidences supporting the conjecture, Aouchiche and Hansen [1] gave counter-examples to the conjecture using AutoGraphiX 2 system, showing that the conjecture is not right when $k > n/2$. In this work, we show that the conjecture is true given the graph contains k vertices of degree $n-1$. Further, it is true among k-trees.

2. Main results

First, we show that Conjecture 1.1 is true given the graph contains k vertices of degree $n-1$.

Theorem 2.1. *For any connected n-vertex graph G containing k vertices of degree* $n-1$, *we have*

$$R(G) \geq \frac{k(n-k)}{\sqrt{k(n-1)}} + \frac{k(k-1)}{2(n-1)}$$

and the equality holds if and only if $G \cong K^{*}_{k,n-k}$.

Proof. Denote by n_i the number of vertices of degree i and by $x_{i,j}$ the number of edges joining vertices of degrees i and j in G, then the minimum degree of G is at least k since G contains k vertices of degree $n-1$. The mathematical description of the problem is as follows:

$$\min R(G) = \min \sum_{k \leq i \leq j \leq n-1} \frac{x_{i,j}}{\sqrt{ij}}$$

subject to:

$$\sum_{\substack{j=k \\ j \neq i}}^{n-1} x_{i,j} + 2x_{i,i} = in_i \quad \text{for } k \leq i \leq n-1;$$

$$n_k + n_{k+1} + \cdots + n_{n-1} = n;$$

$$x_{ij} \leq n_i n_j \quad \text{for } k \leq i < j \leq n-1;$$

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

$x_{i,j}$, n_i are nonnegative integers.