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Graphs with fixed number of pendent vertices and minimal Zeroth-order general Randić index

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ABSTRACT

We investigate the graph with minimal Zeroth-order general Randić index in terms of its order n, pendent number N_1 and cyclomatic number $\gamma \geq 0$. Extremal graphs were completely characterized for cases of $\gamma = 0, 1, 2,$ which can be directly extended for graphs with cyclomatic number $\gamma \geq 3$.

1. Introduction

Throughout this paper, we consider finite undirected graphs without loops and multiple edges. Concepts and notations not defined in this paper are as in standard textbook [1]. Let G be such a graph and let its vertex set be $V(G)$ and edge set $E(G)$, respectively. The numbers of vertices and edges of G are denoted by $n = |V(G)|$ and $m = |E(G)|$, respectively. For a connected graph, the **cyclomatic number** (=number of independent cycles) is equal to $\gamma = m - n + 1$. Recall that graphs with $\gamma = 0, 1, 2$ are referred to as trees, unicyclic graphs and bicyclic graphs, respectively.

A graph invariant is a function on a graph that does not depend on the labeling of its vertices. Hundreds of graph invariants based on distances between the vertices of a graph have been considered in quantitative structure-activity relationship (QSAR) and quantitative structure-property relationship (QSPR) researches. Among the most important degree-based topological indices is the well-known Zeroth-order general Randić index. Let α be a given real number with $\alpha \neq 0$ and $\alpha \neq 1$, the **Zeroth-order general Randić index**, denoted by ${}^0R_\alpha(G)$, was defined by Li and Zheng in [2]:

$$ {}^0R_\alpha(G) = \sum_{u \in V} \deg^\alpha(u), $$

where $\deg(u)$ denotes the degree of vertex u and α is a pertinently chosen real number. This index is a common generalization of the Zeroth-order Randić index [4] and the first Zagreb index (will be given later). Li and Zhao [3] determined the trees with the first three minimum and maximum Zeroth-order general Randić index. In [7] the authors investigated the Zeroth-order general Randić index for molecular (n, m)-graphs, i.e., simple connected graphs with n vertices, m edges and maximum degree at most 4. Zhang and Zhang [5] determined the unicyclic graphs with the first three minimum and maximum Zeroth-order general Randić index. Zhang et al. [6] determined the bicyclic graphs with the first three minimum and maximum Zeroth-order general Randić index. In [8], Hu et al. investigated the Zeroth-order general Randić index for general simple connected (n, m)-graphs and characterized the simple connected (n, m)-graphs with extremal (maximum and minimum) Zeroth-order general Randić index. Li and Shi [9] did some further works on this topic following [8]. In 2009, Cheng and co-workers [10] determined the minimum

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and maximum Zeroth-order general Randić index values of bipartite graphs with a given number of vertices and edges for $\alpha = 2$. In 2013, Su et al. [11] presented several sufficient conditions for graphs to be maximally edge-connected in terms of the Zeroth-order general Randić index, and generalized the results given by Dankelmann et al. [12].

In 1972, Gutman and Trinajstić introduced the **first Zagreb index**:

$$M_1(G) = \sum_{u\in V} \deg^2(u),$$

which can be seen as the special case of the Zeroth-order general Randić index for $\alpha = 2$ and has been considered in connection with certain chemical applications [13,14]. A vast amount of research on the first Zagreb index has been done so far. For details of its mathematical theory see the papers [15–19], the recent contributions could be found in [20–23]. There are many other degree-based topological indices, such as ABC index and Randić index, the interested reader refer to [24–40].

In what follows, we assume that G is connected. Let N_k denote the number of vertices of degree k in graph G. Then, evidently,

$$\sum_{k\geq 1} N_k = n. \tag{1}$$

From the Handshaking Lemma, it immediately follows

$$\sum_{k\geq 1} kN_k = 2m. \tag{2}$$

Thus the Zeroth-order general Randić index of G can be represented as

$$\sum_{k\geq 1} k^{\alpha} N_k = {}^0R_{\alpha}(G). \tag{3}$$

Before processing, we will introduce several more concepts and notations. A vertex of a graph is said to be **pendant** if its neighborhood contains exactly one vertex. Then N_1 is the number of pendent vertices, and the respective graph will be said to be $\boldsymbol{N_1}$**-graph**. Let $\mathcal{G}_{n,m}$ be a class of graphs with n vertices and m edges, and $\boldsymbol{(n, N_1)}$**-graph** is such a graph with n vertices and N_1 pendent vertices. Let x be a real number, denote $\lfloor x \rfloor$ the greatest integer number does not greater than x.

2. General graphs with minimal ${}^0R_{\alpha}$-value

In what follows it will be assumed that the parameter α in Eq. (3) is a positive integer.

Theorem 2.1. *Let G be a connected graph with N_1 pendent vertices, cyclomatic number γ and without vertices of degree 3. Then*

$${}^0R_{\alpha}(G) \geq 4^{\alpha}(\gamma - 1) + (1 + 2^{-1}\cdot 4^{\alpha})N_1. \tag{4}$$

Equality in (4) holds if and only if all non-pendent vertices of G are of degrees 4, provided such graphs exist.

Proof. Multiply Eqs. (1) and (2), respectively by 4^{α} and $-2^{-1}\cdot 4^{\alpha}$, we have

$$\sum_{k\geq 1} 4^{\alpha} N_k = 4^{\alpha} n \text{~~and~~} \sum_{k\geq 1} -2^{-1}\cdot 4^{\alpha} kN_k = -4^{\alpha} m. \tag{5}$$

Adding these equalities to Eq. (3), yields

$${}^0R_{\alpha}(G) = 4^{\alpha}(\gamma - 1) + \sum_{k\geq 1}[4^{\alpha} - 2^{-1}\cdot 4^{\alpha} k + k^{\alpha}]N_k. \tag{6}$$

Let $\Phi(\alpha, k) = 4^{\alpha} - 2^{-1}\cdot 4^{\alpha} k + k^{\alpha}$, which is a polynomial of degree α in the variable k. Simple verifications show the following noteworthy facts:

Fact 1. $\Phi(\alpha, 1) = 1 + 2^{-1}\cdot 4^{\alpha}$ and $\Phi(\alpha, 2) = 2^{\alpha}$ are positive-valued.
Fact 2. $\Phi(\alpha, 4) = 4^{\alpha} - 2^{-1}\cdot 4^{\alpha}\cdot 4 + 4^{\alpha} = 0$.
This suggests that $k = 4$ is a root of the polynomial $\Phi(\alpha, k)$ for all α.
Fact 3. $\Phi(\alpha, k)$ is non-negative-valued for all $k \geq 4$.

In fact, $\Phi(2, k) = k^2 - 8k + 16 = (k - 4)^2$ and $\Phi(3, k) = k^3 - 32k + 64 = (k - 4)(k^2 + 4k - 16)$, which are positive-valued for all $k \geq 5$. On the other hand, if $\alpha \geq 3$,

$$\frac{d\Phi(\alpha, k)}{dk} = \alpha k^{\alpha-1} - 2^{-1}\cdot 4^{\alpha} > 0$$

holds for all $k \geq 5$. This implies that $\Phi(\alpha, k)$ is a monotonically increasing function. Since $\Phi(\alpha, 4) = 0,\ \Phi(\alpha, k) \geq 0$ for $k \geq 4$.

Note that $N_k \geq 0$ for $k \geq 2$, and combining Facts 1–3 we arrive at:

$${}^0R_{\alpha}(G) \geq 4^{\alpha}(\gamma - 1) + (1 + 2^{-1}\cdot 4^{\alpha})N_1. \tag{7}$$

We complete the proof of Theorem 2.1. □