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Research Article

On the modified misbalance rodeg index

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Abstract

Let G be a graph with edge set $E(G)$. Denote by d_u the degree of a vertex u in G. The number $\sum_{vw\in E(G)}\left(\sqrt{d_v}-\sqrt{d_w}\right)^2$ is known as the modified misbalance rodeg (MMR) index of G. The primary goal of this paper is to characterize graphs attaining the maximum and minimum values of the MMR index in the classes of all trees and connected unicyclic graphs with a fixed order. In the case of trees, the path and star graphs attain the minimum and maximum values of the MMR index, respectively. For the case of unicyclic graphs, the cycle graph and the graph formed by inserting an edge in the star graph achieve the minimum and maximum values of the MMR index, respectively.

Keywords: misbalance rodeg index; modified misbalance rodeg index; topological index; tree; unicyclic graph.

2020 Mathematics Subject Classification: 05C05, 05C07, 05C09, 05C35.

1. Introduction

In this paper, only connected graphs are considered. Those graph-theoretical terms that are utilized in this paper without providing their definitions here, can be found in the books [5, 6, 13].

A topological index of a graph G is a numerical quantity associated with G that remains unchanged under graph isomorphism. In order to improve QSPR (quantitative structure-property relationship) studies, Vukičević and Gašperov [18] designed 148 new topological indices and they revealed that only some of them are effective ones; particularly, the misbalance rodeg (MR) index belongs to the class of such effective indices. The MR index for a graph G is defined [18] as

$$MR(G)=\sum_{vw\in E(G)}\left|\sqrt{d_v}-\sqrt{d_w}\right|,$$

where d_v and d_w are the degrees of the vertices v and w of G, respectively, and $E(G)$ denotes the edge set of G. The predicting ability of the MR index for the cases of standard vaporization enthalpy and vaporization enthalpy of octane isomers is significantly well [18].

The primary motivation of the present work comes from the paper [17], where Vukičević and Furtula devised a topological index using the ratios of geometric and arithmetic means of end-vertex degrees of edges of a graph. In the present paper, the difference between arithmetic and geometric means of end-vertex degrees of edges of a graph G is considered; that is,

$$\sum_{vw\in E(G)}\left(\frac{d_v+d_w}{2}-\sqrt{d_vd_w}\right)=\sum_{vw\in E(G)}\frac{\left(\sqrt{d_v}-\sqrt{d_w}\right)^2}{2}. \tag{1}$$

Because of trivial reasons, the factor "1/2" needs to be dropped from the topological index given on the right-hand side of Equation (1). Consequently, the following topological index is considered:

$$MMR(G)=\sum_{vw\in E(G)}\left(\sqrt{d_v}-\sqrt{d_w}\right)^2. \tag{2}$$

Because of the similarity between the definitions of the MR index and the topological index defined via formula (2), it is proposed to call (2) as the modified misbalance rodeg (MMR) index. It found that the absolute value of the correlation between the MR and MMR indices for octane isomers is approximately 0.97. This finding indicates that the predictive ability of the both MMR and MR indices is considerably the same for the case of octane isomers. On the other hand, considering

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all the octane isomers, there are only two groups (each consisting of two elements) of isomers such that all members of each group have the same MMR index; however, there are five groups of isomers (one consisting of four elements, two consisting of three elements, and two consisting of two elements) such that all the members of every group have the same MR index. From this observation, one may expect that the MMR index has better discriminatory ability than that of the MR index. It needs to be noted here that the MMR index is not a new topological index. It was indeed among various topological indices considered in [15], where its chemical applicability was investigated.

The present work may also be regarded as a study of the irregularity in graphs [3]. An irregularity measure (IM) of a (connected) graph G is a topological index fulfilling the property: G is regular if and only if $IM(G) = 0$. Irregularity measures may be useful in QSPR studies [12,15] and in network theory [7,9,10,16]. Albertson's measure of irregularity [2] (see also [1]) is one of the well-investigated irregularity measures; for a graph G, this irregularity measure is defined [2] as follows:

$$A(G) = \sum_{vw \in E(G)} |d_v - d_w|.$$

It is remarked here that the MR and MMR indices are not only irregularity measures but also can be considered variants of Albertson's measure of irregularity. Additional detail about irregularity measures can be found in the recent articles [4,8,11,14].

A graph containing exactly one cycle is known as a unicyclic graph. A graph of order n is referred to as an n-order graph. Denote by P_n, S_n, and C_n the n-order path, star, and cycle graphs, respectively. Let S_n^+ be the graph formed by adding an edge in S_n. Let $\mathbb{T}_n$ and $\mathbb{U}_n$ be the classes of n-order trees and unicyclic graphs. In the present paper, it is proved that P_n and S_n uniquely attain the minimum and maximum values, respectively, of the MMR index in the class $\mathbb{T}_n$ for $n \geq 4$. It is also proved that C_n and S_n^+ uniquely attain the minimum and maximum values, respectively, of the MMR index in the class $\mathbb{U}_n$ for $n \geq 4$.

2. Results

A vertex w of a graph is said to pendent if $d_w = 1$. A pendent edge of a graph is an edge incident with a pendent vertex. The following proposition gives the unique tree attaining the minimum value of the MMR index over the class of all trees of a fixed order.

Proposition 2.1. *If G is a tree of order at least 3, then*

$$MMR(G) \geq 2\left(3 - 2\sqrt{2}\right),$$

with equality if and only if G is the path graph. Particularly, the path graph P_n uniquely achieves the minimum value of the MMR index over the class of all trees of order n for every integer $n \in \{4, 5, 6, \ldots\}$.

Proof. Let $P_E(G)$ be the set of all pendent edges of G. Then, one has

$$\begin{aligned} MMR(G) &= \sum_{uv \in P_E(G)} \left(\sqrt{d_u} - \sqrt{d_v}\right)^2 + \sum_{xy \in E(G) \setminus P_E(G)} \left(\sqrt{d_x} - \sqrt{d_y}\right)^2 \\ &\geq \sum_{uv \in P_E(G)} \left(3 - 2\sqrt{2}\right) + \sum_{xy \in E(G) \setminus P_E(G)} (0) \qquad (3) \\ &= \left(3 - 2\sqrt{2}\right) |P_E(G)| \\ &\geq 2\left(3 - 2\sqrt{2}\right). \qquad (4) \end{aligned}$$

It is observed that the equality in (3) holds if and only if $\max\{d_u, d_v\} = 2$ for every $uv \in P_E(G)$ and $d_x = d_y$ for every $xy \in E(G) \setminus P_E(G)$. Also, the equality in (4) holds if and only if $|P_E(G)| = 2$. □

In order to determine the unique tree attaining the maximum value of the MMR index over the class of all trees of a fixed order, an upper bound on the MMR index for general graphs is derived. For any edge $uv \in E(G)$, note that

$$\left(\sqrt{d_u} - \sqrt{d_v}\right)^2 \leq \left(\sqrt{\Delta} - \sqrt{\delta}\right)^2$$

with equality if and only if $\max\{d_u, d_v\} = \Delta$ and $\min\{d_u, d_v\} = \delta$. This observation yields the next result.

Proposition 2.2. *If G is a graph of size m, maximum degree Δ, and minimum degree δ, then*

$$MMR(G) \le m \left(\sqrt{\Delta} - \sqrt{\delta}\right)^2,$$

where the equality sign holds if and only if $\max\{d_u, d_v\} = \Delta$ *and* $\min\{d_u, d_v\} = \delta$ *for every edge* $uv \in E(G)$.

The next result follows immediately from Proposition 2.2.

Corollary 2.1. *If T is a tree of order n, then*

$$MMR(G) \le (n-1)\left(\sqrt{n-1} - 1\right)^2,$$

where the equality sign holds if and only if T is the star graph S_n. In other words, the star S_n is the unique graph having the maximum value of the MMR index among all trees of order n for every integer $n \in \{4, 5, 6, \ldots\}$.

The next result provides the unique graph attaining the minimum value of the MMR index over the class of all unicyclic graphs of a fixed order.

Proposition 2.3. *For any graph G, it holds that $MMR(G) \ge 0$ with equality if and only if G is regular. In particular, the cycle C_n is the unique graph having the minimum value of the MMR index among all unicyclic graphs of order n for every integer $n \in \{4, 5, 6, \ldots\}$.*

Proof. The result follows from the elementary fact that

$$\left(\sqrt{d_u} - \sqrt{d_v}\right)^2 \ge 0$$

with equality if and only if $d_u = d_v$. □

In the next result, the unique graph attaining the maximum value of the MMR index over the class of all unicyclic graphs of a fixed order is given. For a vertex u of a graph G, define

$$N_G(u) := \{v \in V(G) : \ uv \in E(G)\}.$$

If G is the only graph under consideration, then we simply write $N(u)$.

Theorem 2.1. *The graph form by adding an edge in the star graph S_n (see Figure 2.1) uniquely achieves the maximum value of the MMR index over the class of all unicyclic graphs of order n for every integer $n \in \{4, 5, 6, \ldots\}$.*

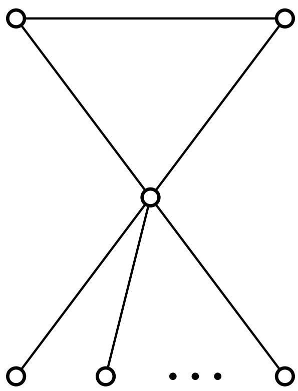

Figure 2.1: The unique graph that achieves the maximum value of the MMR index over the class of all unicyclic graphs of a given order at least 4.

Proof. For $n \in \{4, 5, 6, \ldots\}$, let G be a unicyclic graph of order n. To prove the theorem, it is enough to show that

$$MMR(G) \le (n-3)(\sqrt{n-1} - 1)^2 + 2\left(\sqrt{n-1} - \sqrt{2}\right)^2, \tag{5}$$

with equality if and only if G is the graph formed by adding an edge in the star graph S_n. Inequality (5) is proved by induction on n. For $n = 4$, the result is directly verified. Assume that $n \ge 5$. If $G = C_n$, then the result follows from Proposition 2.3. In what follows, it is assumed that G possesses at least one pendent edge.

Let v_0v be a pendent edge of G where $d_v = t \geq 2$ and v_0 is a pendent vertex. Take $N(v) = \{v_0, \ldots, v_{t-1}\}$ such that $v_0, \ldots, v_{r-1}$ are pendent vertices and $v_r, \ldots, v_{t-1}$ are non-pendent vertices, where $1 \leq r \leq t-1$. Denote by $G - v_0$ the graph formed by deleting the vertex v_0 (and its incident edge). In the rest of the proof, whenever $x \in V(G) \cap V(G - v_0)$, that is $x \in V(G - v_0)$, the notion d_x represents the degree of the vertex x in G not in $G - v_0$. Note that

$$\begin{aligned} MMR(G) - MMR(G - v_0) &= \sum_{i=1}^{t-1}\left[\left(\sqrt{t} - \sqrt{d_{v_i}}\right)^2 - \left(\sqrt{t-1} - \sqrt{d_{v_i}}\right)^2\right] + \left(\sqrt{t} - 1\right)^2 \\ &= (r-1)\left[\left(\sqrt{t}-1\right)^2 - \left(\sqrt{t-1}-1\right)^2\right] + \left(\sqrt{t}-1\right)^2 \\ &\quad + \sum_{i=r}^{t-1}\left[\left(\sqrt{t} - \sqrt{d_{v_i}}\right)^2 - \left(\sqrt{t-1} - \sqrt{d_{v_i}}\right)^2\right] \\ &\leq (r-1)\left[\left(\sqrt{t}-1\right)^2 - \left(\sqrt{t-1}-1\right)^2\right] + \left(\sqrt{t}-1\right)^2 \\ &\quad + (t-r)\left[\left(\sqrt{t}-\sqrt{2}\right)^2 - \left(\sqrt{t-1}-\sqrt{2}\right)^2\right]. \end{aligned} \tag{6}$$

Case 1. When $r = t-1$.
In this case, it holds that $t \leq n-3$ because G is a unicyclic graph. Inequality (6) implies that

$$\begin{aligned} MMR(G) - MMR(G - v_0) &\leq (t-2)\left[\left(\sqrt{t}-1\right)^2 - \left(\sqrt{t-1}-1\right)^2\right] + \left(\sqrt{t}-1\right)^2 \\ &\quad + \left(\sqrt{t}-\sqrt{2}\right)^2 - \left(\sqrt{t-1}-\sqrt{2}\right)^2 \\ &\leq (n-5)\left[\left(\sqrt{n-3}-1\right)^2 - \left(\sqrt{n-4}-1\right)^2\right] + \left(\sqrt{n-3}-1\right)^2 \\ &\quad + \left(\sqrt{n-3}-\sqrt{2}\right)^2 - \left(\sqrt{n-4}-\sqrt{2}\right)^2. \end{aligned} \tag{7}$$

By inductive hypothesis, we have

$$MMR(G - v_0) \leq (n-4)\left(\sqrt{n-2}-1\right)^2 + 2\left(\sqrt{n-2}-\sqrt{2}\right)^2. \tag{8}$$

Since $n \geq 5$, it holds that

$$\begin{aligned} &(n-5)\left[\left(\sqrt{n-3}-1\right)^2 - \left(\sqrt{n-4}-1\right)^2\right] + \left(\sqrt{n-3}-1\right)^2 \\ &+ \left(\sqrt{n-3}-\sqrt{2}\right)^2 - \left(\sqrt{n-4}-\sqrt{2}\right)^2 \\ &+ (n-4)\left(\sqrt{n-2}-1\right)^2 + 2\left(\sqrt{n-2}-\sqrt{2}\right)^2 \\ &< (n-3)\left(\sqrt{n-1}-1\right)^2 + 2\left(\sqrt{n-1}-\sqrt{2}\right)^2, \end{aligned}$$

and thence from (7) and (8) it follows that

$$MMR(G) < (n-3)\left(\sqrt{n-1}-1\right)^2 + 2\left(\sqrt{n-1}-\sqrt{2}\right)^2,$$

as desired.

Case 2. When $r \leq t-2$.
Inequality (6) implies that

$$MMR(G) - MMR(G-v_0) \leq (t-3)\left[\left(\sqrt{t}-1\right)^2 - \left(\sqrt{t-1}-1\right)^2\right] + \left(\sqrt{t}-1\right)^2$$
$$+ 2\left[\left(\sqrt{t}-\sqrt{2}\right)^2 - \left(\sqrt{t-1}-\sqrt{2}\right)^2\right]. \qquad (9)$$

In present case, it holds that $t \leq n-1$ and therefore (9) gives

$$MMR(G) - MMR(G-v_0) \leq (n-4)\left[\left(\sqrt{n-1}-1\right)^2 - \left(\sqrt{n-2}-1\right)^2\right] + \left(\sqrt{n-1}-1\right)^2$$
$$+ 2\left[\left(\sqrt{n-1}-\sqrt{2}\right)^2 - \left(\sqrt{n-2}-\sqrt{2}\right)^2\right]. \qquad (10)$$

Now, from (8) and (10) it follows that

$$MMR(G) \leq (n-3)(\sqrt{n-1}-1)^2 + 2\left(\sqrt{n-1}-\sqrt{2}\right)^2. \qquad (11)$$

Considering the characterization of the equality in (6), (8), (9), and (10), it is concluded that the equality in (11) holds if and only if G is the graph formed by adding an edge in the star graph S_n. □

3. Concluding remarks

A topological index defined using the difference between arithmetic and geometric means of end-vertex degrees of edges of a graph has been studied in this paper. It has been suggested that this index be referred to as the modified misbalance rodeg (MMR) index because it can be considered as a modified version of the misbalance rodeg proposed by Vukičević and Gašperov [18]. It has been proved that the start and path graphs attain the maximum and minimum values of the MMR index, respectively, in the class of all trees with a fixed order of at least 4. It has also been shown that in the class of all unicyclic graphs with a fixed order of at least 4, the cycle graph and the graph formed by inserting an edge in the star graph achieve the minimum and maximum values of the MMR index, respectively. Solving the problem of determining graphs with extremum values of the MMR index among other classes of cyclic graphs of a fixed order is one of the several directions, towards which the present study can be extended.

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