On a vertex-degree-based graph invariant and the multiplicatively weighted Harary index

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Abstract

The *multiplicatively weighted Harary index (H_M-index)* is a new distance-based graph invariant, which was introduced and studied by Deng et al. in [Deng et al., J. Comb. Optim., DOI 10.1007/s10878-013-9698-5]. For a connected graph G, the multiplicatively weighted Harary index of G is defined as $H_M(G) = \sum_{\{u,v\}\subseteq V(G)} \frac{d_G(u)d_G(v)}{d_G(u,v)}$, where $d_G(x)$ denotes the degree of vertex x and $d_G(s,t)$ denotes the distance between vertices s and t in G. In this paper, we first study a new vertex degree-based graph invariant $M_2 - \frac{1}{2}M_1$, where M_1 and M_2 are ordinary Zagreb indices. We characterize the trees attaining maximum value of $M_2 - \frac{1}{2}M_1$ among all trees of given order. As applications, we obtain a new proof of Deng et al.'s results on trees with extremal H_M-index among all trees of given order.

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1 Introduction

Let G be a simple connected graph with vertex set $V(G)$ and edge set $E(G)$. As usual, we use n to denote the order of a graph G, namely, the number of vertices in $V(G)$. For a graph G, we let $d_G(v)$ be the degree of a vertex v in G. A vertex is said to be a pendent vertex if it is of degree one, and is said to be a non-pendent vertex if it is of degree greater than or equal to two. For each $v \in V(G)$, the set of neighbors of the vertex v is denoted by $N_G(v)$. The distance between two vertices u and v in G, namely, the length of the shortest path between u and v is denoted by $d_G(u, v)$. The diameter of a graph G is the maximum distance between any two vertices of G.

One of the oldest and well-studied distance-based graph invariants is the Wiener number $W(G)$, also termed as *Wiener index* in chemical or mathematical chemistry literature. Wiener index is defined [14] as the sum of distances over all unordered vertex pairs in G, namely,

$$W(G) = \sum_{\{u,v\} \subseteq V(G)} d_G(u, v).$$

Dobrynin and Kochetova [6] and Gutman [7] independently introduced a new graph invariant under the name *degree distance* or *Schultz molecular topological index*, which is defined for a nontrivial connected graph G as follows:

$$DD(G) = \sum_{\{u,v\} \subseteq V(G)} (d_G(u) + d_G(v)) d_G(u, v).$$

In [8], Gutman and Klavžar defined *modified Schultz molecular topological index* as follows:

$$DD^*(G) = \sum_{\{u,v\} \subseteq V(G)} d_G(u) d_G(v) d_G(u, v).$$

ular topological index are degree-weight versions of the Wiener index. Another distance-based graph invariant, defined [12] in a fully analogous way to Wiener index, is the *Harary index*, which is equal to the sum of reciprocal distances over all unordered vertex pairs in G, that is,

$$H(G) = \sum_{\{u,v\} \subseteq V(G)} \frac{1}{d_G(u,v)}.$$

Hua and Zhang [9] introduced a new graph invariant named reciprocal degree distance, which can be seen as a degree-weight version of Harary index, that is,

$$RDD(G) = \sum_{\{u,v\} \subseteq V(G)} \frac{d_G(u) + d_G(v)}{d_G(u,v)}.$$

Recently, Alizadeh et. al. [1] defined additively weighted Harary index (the same as the reciprocal degree distance) and was further studied by Deng et al. More precisely, Deng et al. [5] introduced another degree-weight version of Harary index, called *multiplicatively weighted Harary index*, of G, which is defined as

$$H_M(G) = \sum_{\{u,v\} \subseteq V(G)} \frac{d_G(u) d_G(v)}{d_G(u,v)}.$$

In [5], Deng et al. determined the extremal values of the multiplicatively weighted Harary index for trees and unicyclic graphs and characterized the corresponding extremal graphs among all trees and unicyclic graphs of given order, respectively.

In this paper, we aim to give a new proof of Deng et al.'s results on multiplicatively weighted Harary index of trees. We first study a new vertex degree-based graph invariant $M_2 - \frac{1}{2}M_1$, where M_1 and M_2 are ordinary Zagreb indices. We characterize the trees attaining maximum values of $M_2 - \frac{1}{2}M_1$ among all trees of given order. As applications, we obtain a new proof of Deng et al.'s results on trees with extremal H_M-index among all trees of given order. Our method relys on structure analysis and avoids

Before proceeding, we introduce some further notation and terminology. A connected graph is said to be a *tree* if the number of edges in it is equal to its number of vertices minus one. As usual, we denote by P_n the path of order n. Denote by $S_{a,b}$ $(a,\ b \geq 1)$, a double star which is constructed by joining the central vertices of two stars S_{a+1} and S_{b+1}. Other notation and terminology not defined here will conform to those in [3].

2 Extremal value of H_M-index for trees

Till now, hundreds of different graph invariants have been employed in QSAR/QSPR studies, some of which have been proved to be successful (see [13]). Among those successful invariants, there are two invariants called the *first Zagreb index* and the *second Zagreb index* (see [4, 10, 11]), defined as

$$M_1(G) = \sum_{u \in V(G)} (d_G(u))^2 \quad \text{and} \quad M_2(G) = \sum_{uv \in E(G)} d_G(u) d_G(v),$$

respectively.

Recall that the *second Zagreb coindex* of a nontrival graph G, which is defined by Ashrafi et al. [2] as

$$\overline{M}_2(G) = \sum_{uv \notin E(G)} d_G(u) d_G(v).$$

The following result reveals the relationship between the second Zagreb coindex and Zagreb indices.

Lemma 1 ([2]). *If G is a nontrivial graph of size m, then*

$$\overline{M}_2(G) = 2m^2 - M_2(G) - \frac{1}{2} M_1(G).$$

Now, we present a sharp upper bound for multiplicatively weighted Harary index in terms of Zagreb indices.

Proposition 1. *If G is a nontrivial connected graph of size m, then*

$$H_M(G) \leq m^2 + \frac{1}{2}\Big(M_2(G) - \frac{1}{2} M_1(G)\Big) \tag{1}$$

Proof. By the definition of the multiplicatively weighted Harary index and Lemma 1,

$$\begin{aligned} H_M(G) &= \sum_{\{u,v\}\subseteq V(G)} \frac{d_G(u)d_G(v)}{d_G(u,v)} \\ &\leq \sum_{uv\in E(G)} d_G(u)d_G(v) + \frac{1}{2}\sum_{uv\notin E(G)} d_G(u)d_G(v) \\ &= M_2(G) + \frac{1}{2}\overline{M}_2(G) \\ &= M_2(G) + \frac{1}{2}\Big(2m^2 - M_2(G) - \frac{1}{2}M_1(G)\Big) \\ &= m^2 + \frac{1}{2}\Big(M_2(G) - \frac{1}{2}M_1(G)\Big). \end{aligned}$$

It is easy to check the equality case in (1). This completes the proof. □

By Proposition 1, we first investigate upper bounds for $M_2(G)-\frac{1}{2}M_1(G)$ among trees of given order.

2.1 Extremal value of $M_2(G) - \frac{1}{2}M_1(G)$

We first prove a result needed in our following proof.

Lemma 2. *If T is a tree of order $n \geq 3$ and x is a pendent vertex adjacent to a non-pendent vertex y in T such that*

$$\sum_{z\in N_T(y)\setminus\{x\}} d_T(z) = \min\{\sum_{z'\in N_T(y')\setminus\{x'\}} d_T(z') : d_T(x') = 1, d_T(y') \geq 2, \\ x'y' \in E(T)\},$$

then

$$\sum_{z\in N_T(y)\setminus\{x\}} d_T(z) \leq n-2$$

with equality if and only if $T \cong S_n$ or $S_{a,b}\,(a+b=n-2,\ a,\ b\geq 1)$.

Proof. If $T \cong S_n$ or $S_{a,b}$, then

$$\min\{\sum_{z' \in N_T(y')\setminus\{x'\}} d_T(z') : d_T(x') = 1, d_T(y') \geq 2, x'y' \in E(T)\} = n-2,$$

and the result holds readily.

Suppose now that $T \ncong S_n$, $S_{a,b}$. In particular, we have $T \ncong P_3$, P_4. We will show that

$$\min\{\sum_{z' \in N_T(y')\setminus\{x'\}} d_T(z') : d_T(x') = 1, d_T(y') \geq 2, x'y' \in E(T)\} < n-2.$$

If $T \cong P_n (n \geq 5)$, then

$$\min\{\sum_{z' \in N_T(y')\setminus\{x'\}} d_T(z') : d_T(x') = 1, d_T(y') \geq 2, x'y' \in E(T)\} = 2 < n-2,$$

as desired.

So we may assume that $T \ncong P_n (n \geq 5)$. Obviously, T has at least two non-pendent vertices, say u and v, each of which is adjacent to at least a pendent vertex. Assume that the statement of lemma is not true. At the same time, we let x and y be pendent vertices in T which are adjacent to non-pendent vertices u and v, respectively. By our assumption, we have $\sum_{s \in N_T(u)\setminus\{x\}} d_T(s) \geq n-2$ and $\sum_{t \in N_T(v)\setminus\{y\}} d_T(t) \geq n-2$.

Since T is a tree, u and v have at most one common neighbor. When u and v have no common neighbors, since $T \ncong S_{a,b} (a+b = n-2,\ a,\ b \geq 1)$, then T has at least $\frac{1}{2}[2(n-2)+2+d_T(u)+d_T(v)] > n$ edges, a contradiction to the fact that T is a tree. So, we may assume that u and v have exactly one common neighbor, say w. Then T has at least $\frac{1}{2}[2(n-2)+2-d_T(w)+ d_T(u)+d_T(v)+\sum_{z \in N_T(w)\setminus\{u,v\}} d_T(z)] \geq \frac{1}{2}[2(n-2)+2-d_T(w)+d_T(u)+ d_T(v)+d_T(w)-2] \geq \frac{1}{2}[2(n-2)+2-d_T(w)+4+d_T(w)-2] = n$ edges, a contradiction once again.

This completes the proof. $\square$

Using Lemma 2, we are able to characterize trees with the maximum value of $M_2(G) - \frac{1}{2}M_1(G)$.

Theorem 1. *Let T be a nontrivial tree of order n. Then*

$$M_2(T) - \frac{1}{2}M_1(T) \leq \frac{1}{2}(n-1)(n-2) \tag{2}$$

with equality if and only if $T \cong S_n$ or $S_{a,b}\,(a+b=n-2,\ a,\ b \geq 1)$.

Proof. When $n = 2$ or 3, the theorem is obviously true. So, we assume that $n \geq 4$ in the following discussion. We shall complete the proof by induction on n. Assume that the theorem is true for smaller values of n. Choose x to be a pendent vertex adjacent to a non-pendent vertex y in T such that

$$\sum_{z \in N_T(y)\setminus\{x\}} d_T(z) = \min\{ \sum_{z' \in N_T(y')\setminus\{x'\}} d_T(z') : d_T(x') = 1, d_T(y') \geq 2, x'y' \in E(T)\}.$$

By Lemma 2, $\sum_{z \in N_T(y)\setminus\{x\}} d_T(z) \leq n-2$.

Now, we have

$$\begin{aligned}
M_2(T) - \frac{1}{2}M_1(T) &= d_T(y) + M_2(T-x) - \frac{1}{2}M_1(T-x) - \frac{1}{2}(d_T(y))^2 + \\
&\quad \frac{1}{2}(d_{T-x}(y))^2 - \frac{1}{2} + \sum_{yz \in E(T),\, z \neq x} d_T(y)d_T(z) - \\
&\quad \sum_{yz \in E(T),\, z \neq x} (d_T(y)-1)d_T(z) \\
&= d_T(y) - \frac{1}{2} + M_2(T-x) - \frac{1}{2}M_1(T-x) + \\
&\quad \sum_{z \in N_T(y)\setminus\{x\}} d_T(z) - \frac{1}{2}(d_T(y))^2 + \frac{1}{2}(d_{T-x}(y))^2 \\
&\leq d_T(y) - \frac{1}{2} + \frac{1}{2}(n-2)(n-3) + \sum_{z \in N_T(y)\setminus\{x\}} d_T(z) - \\
&\quad \frac{1}{2}(d_T(y))^2 + \frac{1}{2}\Big(d_T(y) - 1\Big)^2 \qquad (3) \\
&\quad \text{(using induction hypothesis)} \\
&= \frac{1}{2}(n-2)(n-3) + \sum_{z \in N_T(y)\setminus\{x\}} d_T(z) \\
&\leq \frac{1}{2}(n-2)(n-3) + (n-2) = \frac{1}{2}(n-1)(n-2). \qquad (4)
\end{aligned}$$

So, we have proved (2). Now, we check the equality case. Suppose that the equality in (2) is attained. Then both equalities in (3) and (4) are attained together. Thus, $M_2(T-x) - \frac{1}{2}M_1(T-x) = \frac{1}{2}(n-2)(n-3)$ and $\sum_{z\in N_T(y)\setminus\{x\}} d_T(z) = n-2$. By induction assumption, $T - x \cong S_{n-1}$ or $S_{c,d}\,(c+d = n-3,\ c,\ d \geq 1)$. Moreover, by Lemma 2, $\sum_{z\in N_T(y)\setminus\{x\}} d_T(z) = n-2$ implies that $T \cong S_n$ or $S_{p,q}\,(p+q = n-2,\ p,\ q \geq 1)$. Summarizing above, we have $T \cong S_n$ or $S_{a,b}\,(a+b = n-2,\ a,\ b \geq 1)$. Conversely, if $T \cong S_n$ or $S_{a,b}\,(a+b = n-2,\ a,\ b \geq 1)$, then the equality in (2) is obviously attained.

This completes the proof. □

2.2 Applications to trees with extremal H_M-index

Now, we using Theorem 1 to deduce result on H_M-index of trees by Deng et al. in [5].

Corollary 1 ([5], **Theorem 8**). *If T is a nontrivial tree of order n, then*

$$H_M(T) \leq \frac{1}{4}(5n^2 - 11n + 6) \tag{5}$$

with equality if and only if $G \cong S_n$.

Proof. By Proposition 1 and Theorem 1, we have

$$\begin{aligned} H_M(T) &\leq (n-1)^2 + \frac{1}{2}\Big(M_2(T) - \frac{1}{2}M_1(T)\Big) && (6)\\ &\leq (n-1)^2 + \frac{1}{4}(n-1)(n-2) && (7)\\ &= \frac{1}{4}(5n^2 - 11n + 6). \end{aligned}$$

Now, we check the equality case in (5). Suppose that the equality in (5) is attained. Then both equalities in (6) and (7) are attained together. Since any double star has diameter three, by Proposition 1 and Theorem 1, $T \cong S_n$. Conversely, if $T \cong S_n$, the equality in (5) is attained. This completes the proof. □

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