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On the reformulated reciprocal sum-degree distance of graph transformations ☆

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ABSTRACT

In this paper, we study a new graph invariant named reformulated reciprocal sum-degree distance ($\overline{R}_t$), which is defined for a connected graph G as $\overline{R}_t(G) = \sum_{\{u,v\}\subseteq V_G}(d_G(u) + d_G(v))\frac{1}{d_G(u,v)+t}$, $t \geq 0$. On the one hand, this new graph invariant $\overline{R}_t$ is a weight version of the t-Harary index, i.e., $H_t(G) = \sum_{\{u,v\}\subseteq V_G}\frac{1}{d_G(u,v)+t}$ defined by Das et al. (2013). On the other hand, it is also the generalized version of reciprocal sum-degree distance of a connected graph, which is defined as $R(G) = \sum_{\{u,v\}\subseteq V_G}(d_G(u) + d_G(v))\frac{1}{d_G(u,v)}$; see Alizadeh et al. (2013) and Hua and Zhang (2012). In this paper we introduce three edge-grafting transformations to study the mathematical properties of $\overline{R}_t(G)$. Using these nice mathematical properties, we characterize the extremal graphs among n-vertex trees with given graphic parameters, such as pendants, matching number, domination number, diameter, and vertex bipartition. Some sharp upper bounds on the reformulated reciprocal sum-degree distance of trees are determined.

1. Introduction

Let G be a simple connected graph with vertex set V_G and edge set E_G. Then $G - v$, $G - uv$ denote the graph obtained from G by deleting vertex $v \in V_G$, or edge $uv \in E_G$, respectively (this notation is naturally extended if more than one vertex or edge is deleted). Similarly, $G + uv$ is obtained from G by adding an edge $uv \notin E_G$. For $v \in V_G$, let $N_G(v)$ (or $N(v)$ for short) denote the set of all the adjacent vertices of v in G and let the degree of v be $d_G(v) = |N_G(v)|$. For a graph G, we let $d_G(u, v)$ be the distance between two vertices u and v in G. Let P_n be the path with n vertices, and let S_n be the star on n vertices. A *pendent path* at v in a graph G is a path in which no vertex other than v is incident with any edge of G outside the path, where the degree of v is at least three. Call v a *pendant vertex* (or a *leaf*) in G, if $d_G(v) = 1$. If $V' \subseteq V_G$, then $G[V']$ denotes the graph on V' whose edges are precisely the edges of G with both ends in V'. We follow [4] for other undefined terminology and notation on graphs.

A single number that can be used to characterize some property of the graph of a molecule is called a topological index, or graph invariant. Topological index is a graph theoretic property that is preserved by isomorphism. The chemical information derived through topological index has been found useful in chemical documentation, isomer discrimination, structure–property correlations, etc. [2]. For quite some time there has been rising interest in the field of computational

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chemistry in topological indices. The interest in topological indices is mainly related to their use in nonempirical quantitative structure–property relationships and quantitative structure–activity relationships. One of the oldest and well-studied distance-based graph invariants associated with a connected graph G is the *Wiener number* $W(G)$, also termed as *Wiener index* in chemical or mathematical chemistry literature, which is defined [29] as the sum of distances over all unordered vertex pairs in G, namely,

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

For more results on Wiener index one may be referred to those in [9,12,23] and their references.

Another distance-based graph invariant, defined [18,25] in a fully analogous manner 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,

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

Recently, Das et al. [7] consider the generalized version of Harary index, namely the *t-Harary index*, which is defined as

$$H_t(G) = \sum_{\{u,v\}\subseteq V_G} \frac{1}{d_G(u, v) + t}, \quad t \geq 0. \tag{1.1}$$

For more results on Harary index, one may be referred to [8,20,24,25,30].

Dobrynin and Kochetova [10] and Gutman [13] independently proposed a *vertex-degree-weighted* version of Wiener index called the *degree distance* or *Schultz molecular topological index*, which is defined for a connected graph G as

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

This graph invariant may be regarded as weighted degree-sum version of Wiener index. One may be referred to [5,6,17,28,27] for degree distance.

Recently, Alizadeh, Iranmanesha and Došlić [1] and Hua and Zhang [15] independently introduced the *reciprocal sum-degree distance* (or, *additively weighted Harary index*) of G, which is defined as

$$R(G) = \sum_{\{u,v\}\subseteq V_G} (d_G(u) + d_G(v))\frac{1}{d_G(u, v)} = \sum_{u\in V_G} d_G(u)\hat{D}_G(u), \tag{1.2}$$

where $\hat{D}_G(u) = \sum_{v\in V_G\setminus\{u\}} \frac{1}{d_G(u,v)}$. For the research development on $R(G)$, one may be referred to [22,26].

Motivated directly from Das et al. [7], Alizadeh et al. [1] and Zhang et al. [15], we introduce here a new graph invariant named the *reformulated reciprocal sum-degree distance*, which is defined as

$$\overline{R}_t(G) = \sum_{\{u,v\}\subseteq V_G} (d_G(u) + d_G(v))\frac{1}{d_G(u, v) + t} = \sum_{u\in V_G} d_G(u)\hat{D}_t(G; u),$$

where $\hat{D}_t(G; u) = \sum_{v\in V_G\setminus\{u\}} \frac{1}{d_G(u,v)+t}$. In view of Eq. (1.1), $\overline{R}_t$ is just the additively weighted t-Harary index; while in view of Eq. (1.2), it is also the generalized version of the reciprocal sum-degree distance of a connected graph G. It is natural and interesting to study the mathematical properties of this novel graph index.

In this paper, we mainly study the mathematical properties of the reformulated reciprocal sum-degree distance under some edge-grafting transformations. Furthermore, extremal properties of the reformulated reciprocal sum-degree distance are also studied for some interesting classes of trees. We organize this paper as follows. In Section 2, we introduce general graph transformations that increase the reformulated reciprocal sum-degree distance for connected graphs. In Section 3, sharp upper bound is established on the maximum reformulated reciprocal sum-degree distance of n-vertex trees with k pendants (resp. matching number, domination number, diameter, given bipartition). The corresponding extremal graphs are identified, respectively.

2. Transformations

In this section, we introduce three edge-grafting transformations on the reformulated reciprocal sum-degree distance of connected graphs. We mainly study the effect of each of these three transformations on the reformulated reciprocal sum-degree distance.

Let G_1 be a simple graph as depicted in Fig. 1, where H_1, H_2 are two connected graphs. Let $G_2 = G_1 - \{v_l x : x \in N_{H_2}(v_l)\} + \{v_1 x : x \in N_{H_2}(v_l)\}$. We call that G_2 is obtained by *α-transformation* on G_1. In particular, if G_1 is a tree, Kelmans [19] used this tree-transformation depicted in Fig. 1 to prove some results on the number of spanning trees of graphs in 1976. Recently, Bollobás and Tyomkyn [3] used this tree-transformation to count the total number of walks (resp. closed walks, paths) of trees. Here we are to show that α-transformation increases the $\overline{R}_t$.