

On Reformulated Reciprocal Product–Degree Distance

Guifu Su¹, Lan Xu^{2,*}, Zhibing Chen³, Ivan Gutman⁴

¹College of Science, Beijing University of Chemical Technology,
Beijing, 100029, P.R. China
gfs@mail.buct.edu.cn

²Department of Mathematics, Changji University,
Changji, 831100, P.R. China
lanxu6400@163.com

³College of Mathematics and Statistics, Shenzhen University,
Guangdong 518060, P.R. China
chenzb@szu.edu.cn

⁴Faculty of Science, University of Kragujevac,
P.O.Box 60, 34000 Kragujevac, Serbia
gutman@kg.ac.rs

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Abstract

We examine the *reformulated reciprocal product–degree distance*, defined for a connected graph G as

$$RDD_{\times}^t = RDD_{\times}^t(G) = \sum_{\substack{\{u,v\} \subseteq V(G) \\ u \neq v}} \frac{\delta_G(u)\delta_G(v)}{d_G(u,v) + t}, t \geq 0,$$

where $\delta_G(u)$ is the degree of the vertex u , whereas $d_G(u, v)$ is the distance between vertices u and v . RDD_{\times}^t is the generalization of the earlier considered t -Harary index and of the reciprocal product–degree distance.

We first show that RDD_{\times}^t is monotonic on two transformations, and then determine its extremal values. We then determine the maximum RDD_{\times}^t of unicyclic graphs with given girth. In addition, we present several relationships between the reciprocal sum–degree distance and the reciprocal product–degree distance. The corresponding extremal graphs are also characterized.

*Corresponding author

1 Introduction

Let $G = (V(G), E(G))$ be a simple connected graph with $n = |V(G)|$ vertices and $m = |E(G)|$ edges. The *degree* of a vertex $v \in V(G)$ is the number $\delta_G(v)$ of edges incident to v . The *distance* $d_G(u, v)$ between two vertices u and v in a connected graph G is the number of edges in a shortest path joining u and v . When the graph is clear from the context, we omit the subscript G from the notation. For standard graph-theoretic notation and terminology the reader is referred to [5, 6].

A single number, calculated from the underlying molecular graph, that can be used to characterize some property of a molecule is called a *topological index*. Topological indices have been found to be useful in establishing relations between the structure and the properties of chemical substances. One of the oldest and well-studied distance-based topological index is the *Wiener number*, also termed as *Wiener index*, defined as

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

This index was first time introduced by Wiener more than 60 years ago [41]. Initially, the Wiener index was considered as a molecular-structure descriptor used in chemical applications, but soon it attracted the interest of “pure” mathematicians [17, 18]; for details and additional references see the reviews [13, 44].

In order to overcome the inconsistency caused by large contributions of pairs of distance vertices, the sum of reciprocal values of distances was put forward in [26, 36] and named *Harary index*:

$$H = H(G) = \sum_{\{u,v\} \subseteq V(G)} \frac{1}{d_G(u, v)}. \quad (2)$$

Das et. al. [10] considered the generalized version of Harary index, namely the *t-Harary index*, defined as

$$H_t = H_t(G) = \sum_{\{u,v\} \subseteq V(G)} \frac{1}{d_G(u, v) + t}, \quad t \geq 0. \quad (3)$$

For results on Harary index see [11, 32, 33, 36, 42].

In 1994, Dobrynin and Kochetova [14] and one of the present authors [22] independently introduced a vertex-degree-weighted version of the Wiener index called *degree distance* or which is defined for a connected graph G as

$$DD_+ = DD_+(G) = \sum_{\{u,v\} \subseteq V(G)} [\delta_G(u) + \delta_G(v)] d_G(u, v). \quad (4)$$

In what follows, we shall refer to it as to the *sum-degree distance*. This graph invariant may be regarded as a weighted version of the Wiener index. For details on its theory see [1, 7, 16, 25, 27, 40] and the references cited therein.

The multiplicative variant of the degree distance put forward in [22] and is nowadays usually called called *Gutman index*. We shall, however, call it *product-degree distance*. It is defined as

$$DD_{\times} = DD_{\times}(G) = \sum_{\{u,v\} \subseteq V(G)} [\delta_G(u) \delta_G(v)] d_G(u, v). \quad (5)$$

This graph invariant can be viewed as a weighted degree-product version of the Wiener index. The interested readers may consult [4, 21, 28, 34, 35, 43] and the references quoted therein.

Noting that the sum-degree distance is a degree-weighted version of the Wiener index, and bearing in mind the relation between Wiener and Harary indices, Alizadeh et al. [2] and Hua et al. [24] introduced the *reciprocal sum-degree distance* or *additively weighted Harary index* as

$$RDD_+ = RDD_+(G) = \sum_{\substack{\{u,v\} \subseteq V(G) \\ u \neq v}} \frac{\delta_G(u) + \delta_G(v)}{d_G(u, v)}. \quad (6)$$

Some basic mathematical properties of this index were established in [29, 30, 39].

By replacing the additive weighting by multiplicative one, one arrives at the *reciprocal product-degree distance* [2]:

$$RDD_{\times} = RDD_{\times}(G) = \sum_{\substack{\{u,v\} \subseteq V(G) \\ u \neq v}} \frac{\delta_G(u) \delta_G(v)}{d_G(u, v)}. \quad (7)$$

For the research of this graph invariant see [3, 12, 38].

Recently, Li et al. [31] introduced a further graph invariant, the *reformulated reciprocal sum-degree distance*, defined as

$$RDD_+^t = RDD_+^t(G) = \sum_{\substack{\{u,v\} \subseteq V(G) \\ u \neq v}} \frac{\delta_G(u) + \delta_G(v)}{d_G(u, v) + t}, \quad t \geq 0. \quad (8)$$

In view of Eq. (3), RDD_+^t is just the additively weighted t -Harary index, whereas in view of Eq. (6), it is also the generalized version of the reciprocal sum-degree distance.

The graph invariants, defined by Eqs. (1)–(8), can be arranged as in the following table.

W	DD_+	DD_\times
H	RDD_+	RDD_\times
H_t	RDD_+^t	\bullet

From this table it is immediately seen that one more such invariant should be placed in it. This is the *reformulated reciprocal product-degree distance* [37], defined as

$$RDD_\times^t = RDD_\times^t(G) = \sum_{\substack{\{u,v\} \subseteq V(G) \\ u \neq v}} \frac{\delta_G(u) \delta_G(v)}{d_G(u,v) + t}, \quad t \geq 0. \quad (9)$$

In view of Eq. (3), RDD_\times^t is just the multiplicatively weighted t -Harary index, whereas in view of Eq. (7), it is also the generalized version of the reciprocal product-degree distance.

W	DD_+	DD_\times
H	RDD_+	RDD_\times
H_t	RDD_+^t	RDD_\times^t

In this paper, we first show that the reformulated reciprocal product-degree distance is monotonic on two transformations, and then determine the extremal values of this new invariant for general graphs and trees. In the third part, we investigate the extremal values of the reformulated reciprocal product-degree distance for unicyclic graphs with given girth. The corresponding extremal graphs are also characterized.

2 Graphs with maximum and minimum RDD_\times^t

In this section, we determine the minimum and maximum value of the reformulated reciprocal product-degree distance for trees. Our first result pertains to the following transformation.

Lemma 1. *Let G_0 be a graph with at least two vertices, and $P = v_1v_2v_3 \cdots v_r$ a path of length $r - 1 \geq 2$. If G (resp. G') is the graph obtained by identifying a vertex v_0 in G_0 to v_k (resp. v_{k-1}) in P , $2 \leq k \leq \frac{r}{2}$, then $RDD_\times^t(G') < RDD_\times^t(G)$.*

Proof. Let $T = \{v_1, v_2, \dots, v_r\}$ and let G_0 denote the subgraph of G induced by the vertex set $V(G) - T$. From the definition of $RDD_{\times}^t(G)$, we have

$$\begin{aligned} RDD_{\times}^t(G) &\leq \left[\sum_{x,y \in V(G_0) - v_0} + \sum_{x,y \in T - \{v_k, v_{k-1}\}} + \sum_{\substack{x \in V(G_0) - v_0 \\ y \in T - \{v_k, v_{k-1}\}}} \right] \frac{\delta(x)\delta(y)}{d(x,y) + t} \\ &+ \delta(v_k) \left[\sum_{x \in V(G_0) - v_0} \frac{\delta(x)}{d(x, x_0) + t} + \sum_{x \in T - v_k} \frac{\delta(x)}{d(x, v_{k-1}) + t} \right] \\ &+ \delta(v_{k-1}) \left[\sum_{x \in V(G_0) - v_0} \frac{\delta(x)}{d(x, x_0) + 1 + t} + \sum_{x \in T - \{v_k, v_{k-1}\}} \frac{\delta(x)}{d(x, v_{k-1}) + t} \right]. \end{aligned}$$

Let $\alpha^t = \alpha(x, t) = d_{G_0}(x, v_0) + t$ for $x \in V(G_0) - v_0$ and $H_n^t = \sum_{k=1}^n \frac{1}{k+t}$ be the new version of the n -th harmonic number. For simplicity, we distinguish the following two cases depending on k .

Case 1. $k > 2$

After using the transformation $G \Rightarrow G'$ repeatedly, the degree of v_{k-1} increases by $\delta_{G_0}(v_0)$, whereas the degree of the vertex v_k decreases by $\delta_{G_0}(v_0)$. During the transformation, for pairs $x, y \in V(G_0) - v_0$ or $x, y \in T - \{v_k, v_{k-1}\}$, the contribution $\frac{\delta(x)\delta(y)}{d(x,y)+t}$ does not change. It remains to analysis the following three possible contributions to the reformulated reciprocal product-degree distance of G .

- For $x \in V(G_0) - v_0$ and $y \in T - \{v_k, v_{k-1}\}$, we have

$$\begin{aligned} A_1 &= \sum_{\substack{x \in V(G_0) - v_0 \\ y \in T - \{v_k, v_{k-1}\}}} \frac{\delta(x)\delta(y)}{d(x,y) + t} \\ &= \sum_{x \in V(G_0) - v_0} \delta(x) \left[\frac{1}{\alpha^t + k - 1 + t} + 2(H_{\alpha^t+k-2}^t - H_{\alpha^t+1}^t) \right. \\ &\quad \left. + 2(H_{\alpha^t+r-k-1}^t - H_{\alpha^t}^t) + \frac{1}{\alpha^t + r - k + t} \right]. \end{aligned}$$

whereas in the graph G' , it becomes

$$\begin{aligned} B_1 &= \sum_{\substack{x \in V(G_0) - v_0 \\ y \in T - \{v_k, v_{k-1}\}}} \frac{\delta(x)\delta(y)}{d(x,y) + t} \\ &= \sum_{x \in V(G_0) - v_0} \delta(x) \left[\frac{1}{\alpha^t + k - 2 + t} + 2(H_{\alpha^t+k-3}^t - H_{\alpha^t}^t) \right. \end{aligned}$$

$$+ 2(H_{\alpha^t+r-k}^t - H_{\alpha^t+1}^t) + \frac{1}{\alpha^t+r-k+1+t} \Big].$$

- For the vertex v_k in the graph G , we have

$$\begin{aligned} A_2 &= \delta(v_k) \left[\sum_{x \in V(G_0)-v_0} \frac{\delta(x)}{d(x, v_0) + t} + \sum_{x \in T-v_k} \frac{\delta(x)}{d(x, v_k) + t} \right] \\ &= (\delta(v_0) + 2) \left[\frac{1}{k-1+t} + 2H_{k-2}^t + 2H_{r-k-1}^t + \frac{1}{r-k+t} + \sum_{x \in V(G_0)-v_0} \frac{\delta(x)}{\alpha^t} \right]. \end{aligned}$$

whereas in the graph G' , it becomes

$$\begin{aligned} B_2 &= \delta(v_k) \left[\sum_{x \in V(G_0)-v_0} \frac{\delta(x)}{d(x, v_0) + 1 + t} + \sum_{x \in T-v_k} \frac{\delta(x)}{d(x, v_k) + t} \right] \\ &= 2 \left[\frac{1}{k-1+t} + 2(H_{k-2}^t - H_1^t) + (\delta(v_0) + 2) + 2H_{r-k-1}^t \right. \\ &\quad \left. + \frac{1}{r-k+t} + \sum_{x \in V(G_0)-v_0} \frac{\delta(x)}{\alpha^t + 1} \right]. \end{aligned}$$

- For the vertex v_{k-1} in the graph G ,

$$\begin{aligned} A_3 &= \delta(v_{k-1}) \left[\sum_{x \in V(G_0)-v_0} \frac{\delta(x)}{d(x, v_0) + 1 + t} + \sum_{x \in T-\{v_{k-1}, v_k\}} \frac{\delta(x)}{d(x, v_{k-1}) + t} \right] \\ &= 2 \left[\frac{1}{k-2+t} + 2H_{k-3}^t + 2(H_{r-k}^t - H_1^t) + \frac{1}{r-k+1+t} + \sum_{x \in V(G_0)-v_0} \frac{\delta(x)}{\alpha^t + 1} \right]. \end{aligned}$$

whereas in the graph G' , it becomes

$$\begin{aligned} B_3 &= \delta(v_{k-1}) \left[\sum_{x \in V(G_0)-v_0} \frac{\delta(x)}{d(x, v_0) + t} + \sum_{x \in T-\{v_{k-1}, v_k\}} \frac{\delta(x)}{d(x, v_{k-1}) + t} \right] \\ &= (\delta(v_0) + 2) \left[\frac{1}{k-2+t} + 2H_{k-3}^t + 2(H_{r-k}^t - H_1^t) + \frac{1}{r-k+1+t} + \sum_{x \in V(G_0)-v_0} \frac{\delta(x)}{\alpha^t} \right]. \end{aligned}$$

Hence,

$$\begin{aligned} RDD_{\times}^t(G) - RDD_{\times}^t(G') &= (A_1 + A_2 + A_3) - (B_1 + B_2 + B_3) \\ &= \sum_{x \in V(G_0)-v_0} \delta(x) \left[\frac{1}{\alpha + k - 1 + t} + \frac{1}{\alpha + k - 2 + t} \right] \end{aligned}$$

$$- \left[\frac{1}{\alpha + r - k + t} - \frac{1}{\alpha + r - k + 1 + t} \right] + \delta(v_0) \left[\frac{1}{k - 1 + t} + \frac{1}{k - 2 + t} - \frac{1}{r - k + t} - \frac{1}{r - k + 1 + t} \right] > 0.$$

The inequality holds since for $k \leq \frac{r}{2}$, we have

$$\left[\frac{1}{\alpha + k - 1 + t} + \frac{1}{\alpha + k - 2 + t} - \frac{1}{\alpha + r - k + t} - \frac{1}{\alpha + r - k + 1 + t} \right] > 0, \\ \left[\frac{1}{k - 1 + t} + \frac{1}{k - 2 + t} - \frac{1}{r - k + t} - \frac{1}{r - k + 1 + t} \right] > 0.$$

Case 2. $k = 2$

By the similar approach as in the previous case, it should consider three possibilities.

In the graph G , let

$$A_1 = \sum_{\substack{x \in V(G_0) - v_0 \\ y \in T - \{v_k, v_{k-1}\}}} \frac{\delta(x)\delta(y)}{d(x, y) + t} = \sum_{x \in V(G_0) - v_0} \delta(x) \left[\frac{1}{\alpha^t + r - 2 + t} + 2(H_{\alpha^t + r - 3}^t - H_{\alpha^t}^t) \right]. \\ A_2 = \delta(v_k) \left[\sum_{x \in V(G_0) - v_0} \frac{\delta(x)}{d(x, v_0) + t} + \sum_{x \in T - v_k} \frac{\delta(x)}{d(x, v_k) + t} \right] \\ = (\delta(v_0) + 2) \left[\frac{1}{1 + t} + 2H_{r-3}^t + \frac{1}{r - 2 + t} + \sum_{x \in V(G_0) - v_0} \frac{\delta(x)}{\alpha^t} \right]. \\ A_3 = \delta(v_{k-1}) \left[\sum_{x \in V(G_0) - v_0} \frac{\delta(x)}{d(x, v_0) + t} + \sum_{x \in T - \{v_{k-1}, v_k\}} \frac{\delta(x)}{d(x, v_{k-1}) + t} \right] \\ = 2 \left(H_{r-2}^t - \frac{1}{1 + t} \right) + \frac{1}{r - 1 + t} + \sum_{x \in V(G_0) - v_0} \frac{\delta(x)}{\alpha^t + 1}.$$

In the graph G' , each of these becomes

$$B_1 = \sum_{\substack{x \in V(G_0) - v_0 \\ y \in T - \{v_k, v_{k-1}\}}} \frac{\delta(x)\delta(y)}{d(x, y) + t} = \sum_{x \in V(G_0) - v_0} \delta(x) \left[\frac{1}{\alpha^t + r - 1 + t} + 2(H_{\alpha^t + r - 2}^t - H_{\alpha^t + 1}^t) \right]. \\ B_2 = \delta(v_k) \left[\sum_{x \in V(G_0) - v_0} \frac{\delta(x)}{d(x, v_0) + t} + \sum_{x \in T - v_k} \frac{\delta(x)}{d(x, v_k) + t} \right] \\ = 2 \left[\frac{\delta(v_0) + 1}{1 + t} + 2H_{r-3}^t + \frac{1}{r - 2 + t} + \sum_{x \in V(G_0) - v_0} \frac{\delta(x)}{\alpha^t + 1} \right].$$

$$\begin{aligned}
 B_3 &= \delta(v_{k-1}) \left[\sum_{x \in V(G_0) - v_0} \frac{\delta(x)}{d(x, v_0) + t} + \sum_{x \in T - \{v_{k-1}, v_k\}} \frac{\delta(x)}{d(x, v_{k-1}) + t} \right] \\
 &= (\delta(v_0) + 1) \left[2 \left(H_{r-2}^t - \frac{1}{1+t} \right) + \frac{1}{r-1+t} + \sum_{x \in V(G_0) - v_0} \frac{\delta(x)}{\alpha^t} \right].
 \end{aligned}$$

From the above it follows

$$\begin{aligned}
 RDD_{\times}^t(G) - RDD_{\times}^t(G') &= (A_1 + A_2 + A_3) - (B_1 + B_2 + B_3) \\
 &= \sum_{x \in V(G_0) - v_0} \delta(x) \left[\frac{2}{\alpha^t + 1 + t} - \frac{1}{\alpha^t + r - 2 + t} - \frac{1}{\alpha^t + r - 1 + t} \right] \\
 &+ \delta(v_0) \left[\frac{2}{1+t} - \frac{1}{r-2+t} - \frac{1}{r-1+t} \right] + 2 \left[H_{r-3}^t - \frac{\delta(v_0)}{1+t} \right] \\
 &+ \sum_{x \in V(G_0) - v_0} \delta(x) \left[\frac{1}{\alpha^t + t} - \frac{1}{\alpha^t + 1 + t} \right] > 0.
 \end{aligned}$$

We have exhausted all the cases, so the proof is completed. ■

Repeatedly using Lemma 1, one immediately obtains:

Theorem 1. *Let T be a tree with $n \geq 2$ vertices, then $RDD_{\times}^t(P_n) \leq RDD_{\times}^t(T)$, with equality if and only if T is isomorphic to P_n .*

Theorem 2. *Let G be a connected graph with n vertices, then $RDD_{\times}^t(P_n) \leq RDD_{\times}^t(G) \leq RDD_{\times}^t(K_n)$.*

Proof. Let T be a spanning tree of G . Since adding an edge to a graph will increase the degrees of its vertices and decrease the distances between some vertices, it follows that $RDD_{\times}^t(T) \leq RDD_{\times}^t(G) \leq RDD_{\times}^t(K_n)$. In view of Theorem 1, we have $RDD_{\times}^t(P_n) \leq RDD_{\times}^t(T)$, as desired. ■

In order to find the upper bound of the reformulated reciprocal product-degree distance for trees, we need the following:

Lemma 2. *Let v be a vertex of degree $p + 1$ of the graph G , such that vv_1, vv_2, \dots, vv_p are pendent edges incident with v , and u is the neighbor of v distinct from*

v_1, v_2, \dots, v_p . Let \widehat{G} be the graph obtained from G by removing edges vv_1, vv_2, \dots, vv_p and adding new edges uv_1, uv_2, \dots, uv_p . Then $RDD_{\times}^t(G) \leq RDD_{\times}^t(\widehat{G})$, with equality if and only if G is a star with v as its center.

Proof. Let $T = \{v, v_1, v_2, \dots, v_p\}$ and H denote the subgraph of G induced by the vertex set $V(G) \setminus T$. From the definition of $RDD_{\times}^t(G)$, we have

$$\begin{aligned} RDD_{\times}^t(G) &= \left[\sum_{x,y \in H-u} + \sum_{x,y \in T-v} + \sum_{\substack{x \in H-u \\ y \in T-v}} \right] \frac{\delta(x)\delta(y)}{d(x,y)+t} \\ &+ \delta(u) \left[\sum_{x \in H-u} \frac{\delta(x)}{d(x,u)+t} + \sum_{x \in T-v} \frac{\delta(x)}{d(x,u)+t} \right] \\ &+ \delta(v) \left[\sum_{x \in H-u} \frac{\delta(x)}{d(x,v)+t} + \sum_{x \in T-v} \frac{\delta(x)}{d(x,v)+t} \right] + \frac{\delta(u)\delta(v)}{d(u,v)+t}. \end{aligned}$$

The transformation $G \Rightarrow \widehat{G}$, implies the following facts.

-- The degree of the vertex u increases by p after using the transformation, whereas the degree of the vertex v decreases by p .

-- The distance between v_i and v_j for $i \neq j$ does not change at all.

-- The distance between v_i and v increases by one, whereas the distance between v_i , $1 \leq i \leq p$, and other vertices decreases by one.

-- For $x, y \in H - u$ and $x, y \in T - v$, the contribution $\sum \frac{\delta(x)\delta(y)}{d(x,y)+t}$ does not change.

It remains to consider the following three contributions to the reformulated reciprocal product-degree distance of G .

- For $x \in H - u$ and $y \in T - v$ in the graph G ,

$$A_1 = \sum_{\substack{x \in H-u \\ y \in T-v}} \frac{\delta(x)\delta(y)}{d(x,y)+t} = \sum_{\substack{x \in H-u \\ y \in T-v}} \frac{\delta(x)}{d(x,y)+t}.$$

whereas in the graph \widehat{G} ,

$$B_1 = \sum_{\substack{x \in H-u \\ y \in T-v}} \frac{\delta(x)\delta(y)}{d(x,y)+t} = \sum_{\substack{x \in H-u \\ y \in T-v}} \frac{\delta(x)}{d(x,y)-1+t}.$$

- For the vertex u in the graph G ,

$$\begin{aligned} A_2 &= \delta(u) \left[\sum_{x \in H-u} \frac{\delta(x)}{d(x,u)+t} + \sum_{x \in T-v} \frac{\delta(x)}{d(x,u)+t} \right] \\ &= \delta(u) \sum_{x \in H-u} \frac{\delta(x)}{d(x,u)+t} + \frac{p\delta(u)}{2+t}. \end{aligned}$$

whereas in \widehat{G} , it becomes

$$\begin{aligned} B_2 &= \sum_{x \in H-u} \frac{(\delta(u) + p)\delta(x)}{d(x, u) + t} + \sum_{x \in T-v} \frac{(\delta(u) + p)\delta(x)}{d(x, u) + t} \\ &= \delta(u) \sum_{x \in H-u} \frac{\delta(x)}{d(x, u) + t} + p \sum_{x \in H-u} \frac{\delta(x)}{d(x, u) + t} + \frac{p\delta(u) + p^2}{1 + t}. \end{aligned}$$

- For the vertex v in the graph G ,

$$\begin{aligned} A_3 &= \delta(v) \left[\sum_{x \in H-u} \frac{\delta(x)}{d(x, v) + t} + \sum_{x \in T-v} \frac{\delta(x)}{d(x, v) + t} + \frac{\delta(u)}{d(u, v) + t} \right] \\ &= (p + 1) \sum_{x \in H-u} \frac{\delta(x)}{d(x, u) + 1 + t} + \frac{p(p + 1)}{1 + t} + \frac{(p + 1)\delta(u)}{1 + t} \\ &= p \sum_{x \in H-u} \frac{\delta(x)}{d(x, u) + 1 + t} + \sum_{x \in H-u} \frac{\delta(x)}{d(x, u) + 1 + t} + \frac{p^2 + p}{1 + t} + \frac{p\delta(u) + \delta(u)}{1 + t}. \end{aligned}$$

whereas in \widehat{G} , it becomes

$$\begin{aligned} B_3 &= \sum_{x \in H-u} \frac{\delta(x)}{d(x, v) + t} + \sum_{x \in T-v} \frac{\delta(x)}{d(x, v) + t} + \frac{\delta(u) + p}{d(u, v) + t} \\ &= \sum_{x \in H-u} \frac{\delta(x)}{d(x, u) + 1 + t} + \frac{p}{2 + t} + \frac{\delta(u) + p}{1 + t}. \end{aligned}$$

Note that the vertex u has at least $\delta(u) - 1$ neighbors $x \in H - u$, it immediately follows

that $\sum_{x \in H-u} \frac{\delta(x)}{(d(x, u) + t)(d(x, u) + 1 + t)} \geq \frac{\delta(u) - 1}{2 + t}$. Hence, we have

$$\begin{aligned} RDD_{\times}^t(\widehat{G}) - RDD_{\times}^t(G) &= (B_1 - A_1) + (B_2 - A_2) + (B_3 - A_3) \\ &= \left[\sum_{\substack{x \in H-u \\ y \in T-v}} \frac{\delta(x)}{d(x, y) - 1 + t} - \sum_{\substack{x \in H-u \\ y \in T-v}} \frac{\delta(x)}{d(x, y) + t} \right] \\ &+ \left[p \sum_{x \in H-u} \frac{\delta(x)}{d(x, u) + t} + \frac{p\delta(u) + p^2}{1 + t} - \frac{p\delta(u)}{2 + t} \right] \\ &+ \left[\frac{p}{2 + t} - \frac{p\delta(u) + p^2}{1 + t} - p \sum_{x \in H-u} \frac{\delta(x)}{d(x, u) + 1 + t} \right] \\ &= \sum_{\substack{x \in H-u \\ y \in T-v}} \frac{\delta(x)}{(d(x, y) - 1 + t)(d(x, y) + t)} \\ &+ \left[p \sum_{x \in H-u} \frac{\delta(x)}{(d(x, y) + t)(d(x, y) + 1 + t)} - \frac{(\delta(u) - 1)p}{2 + t} \right] \geq 0. \end{aligned}$$

The equality holds if and only if H contains only one vertex u , i.e., G is a star with v as its center. ■

For a tree T on n vertices, if T is not isomorphic to S_n , then T can be transformed into S_n by using Lemma 2 repeatedly. Hence, we have

Theorem 3. *Let T be a tree on n vertices, then $RDD_{\times}^t(T) \leq RDD_{\times}^t(S_n)$ with equality if and only if T is isomorphic to S_n .*

3 Unicyclic graphs with maximum RDD_{\times}^t

In this section we focus on a special class of unicyclic graphs. Let $U_{n,k}$ be the unicyclic graph of order $n \geq 3$ with girth $k \geq 3$ obtained from C_k by adding $n - k$ pendent vertices to a vertex of C_k .

Lemma 3. *Let u and v be two vertices of a graph H . We use G to denote the graph obtained from H by attaching p pendent vertices u_1, u_2, \dots, u_p and q pendent vertices v_1, v_2, \dots, v_q to u and v , respectively. Assume that*

$$\begin{aligned} G_1 &= G - \{vv_1, vv_2, \dots, vv_q\} + \{uv_1, uv_2, \dots, uv_q\} \\ G_2 &= G - \{uu_1, uu_2, \dots, uu_p\} + \{vu_1, vu_2, \dots, vu_p\}. \end{aligned}$$

Then $RDD_{\times}^t(G) < RDD_{\times}^t(G_1)$ or $RDD_{\times}^t(G) < RDD_{\times}^t(G_2)$.

Proof. For convenience, let $A = \{u_1, u_2, \dots, u_s\}$, $B = \{v_1, v_2, \dots, v_t\}$ and $d_H(u, v) = \ell$. From G to G_1 , for any pair of vertices x, y satisfying $x, y \in H - u - v$ or $x, y \in A$ or $x, y \in B$ or $x \in A$ and $y \in H - u - v$, the contribution $\sum_{x,y} \frac{\delta(x)\delta(y)}{d(x,y)+t}$ does not change. Hence

$$\begin{aligned} RDD_{\times}^t(G) &= \left[\sum_{x,y \in H-u-v} + \sum_{x,y \in A} + \sum_{x,y \in B} + \sum_{\substack{x \in A \\ y \in H-u-v}} \right] \frac{\delta(x)\delta(y)}{d(x,y)+t} \\ &+ \sum_{\substack{x \in A \\ y \in B}} \frac{\delta(x)\delta(y)}{d(x,y)+t} + \sum_{\substack{x \in H-u-v \\ y \in B}} \frac{\delta(x)\delta(y)}{d(x,y)+t} \\ &+ \delta(u) \left[\sum_{x \in H-u-v} \frac{\delta(x)}{d(x,u)+t} + \sum_{x \in A} \frac{\delta(x)}{d(x,u)+t} + \sum_{x \in B} \frac{\delta(x)}{d(x,u)+t} \right] \end{aligned}$$

$$\begin{aligned}
 & + \delta(v) \left[\sum_{x \in H-u-v} \frac{\delta(x)}{d(x, v) + t} + \sum_{x \in A} \frac{\delta(x)}{d(x, v) + t} + \sum_{x \in B} \frac{\delta(x)}{d(x, v) + t} \right] \\
 & + \frac{\delta(u)\delta(v)}{d(u, v) + t}. \tag{10}
 \end{aligned}$$

It is routine to check that

$$\begin{aligned}
 RDD_{\times}^t(G) &= \left[\sum_{x, y \in H-u-v} + \sum_{x, y \in A} + \sum_{x, y \in B} + \sum_{\substack{x \in A \\ y \in H-u-v}} \right] \frac{\delta(x)\delta(y)}{d(x, y) + t} \\
 &+ \frac{pq}{\ell + 2 + t} + q \sum_{x \in H-u-v} \frac{\delta(x)}{d(x, v) + 1 + t} \\
 &+ (p + \delta_H(u)) \left[\sum_{x \in H-u-v} \frac{\delta(x)}{d(x, u) + t} + \frac{p}{1 + t} + \frac{q}{\ell + 1 + t} \right] \\
 &+ (q + \delta_H(v)) \left[\sum_{x \in H-u-v} \frac{\delta(x)}{d(x, v) + t} + \frac{q}{1 + t} + \frac{p}{\ell + 1 + t} \right] \\
 &+ \frac{(p + \delta_H(u))(q + \delta_H(v))}{\ell + t}.
 \end{aligned}$$

Similarly,

$$\begin{aligned}
 RDD_{\times}^t(G_1) &= \left[\sum_{x, y \in H-u-v} + \sum_{x, y \in A} + \sum_{x, y \in B} + \sum_{\substack{x \in A \\ y \in H-u-v}} \right] \frac{\delta(x)\delta(y)}{d(x, y) + t} + \frac{pq}{2 + t} \\
 &+ q \sum_{x \in H-u-v} \frac{\delta(x)}{d(x, u) + 1 + t} + (p + q + \delta_H(u)) \\
 &\times \left[\sum_{x \in H-u-v} \frac{\delta(x)}{d(x, u) + t} + \frac{p}{1 + t} + \frac{q}{1 + t} \right] \\
 &+ \delta_H(v) \left[\sum_{x \in H-u-v} \frac{\delta(x)}{d(x, v) + t} + \frac{p}{\ell + 1 + t} + \frac{q}{\ell + 1 + t} \right] \\
 &+ \frac{\delta_H(v)(p + q + \delta_H(u))}{\ell + t}.
 \end{aligned}$$

Combing the previous two equalities, we get

$$\begin{aligned}
 RDD_{\times}^t(G_1) - RDD_{\times}^t(G) &= q \sum_{x \in H-u-v} \delta(x) \left[\frac{d(x, v) - d(x, u)}{(d(x, u) + 1 + t)(d(x, v) + 1 + t)} \right] \\
 &+ q \sum_{x \in H-u-v} \delta(x) \left[\frac{d(x, v) - d(x, u)}{(d(x, v) + t)(d(x, u) + t)} \right]
 \end{aligned}$$

$$\begin{aligned}
 &+ \frac{2q\ell(\delta_H(u) - \delta_H(v))}{(1+t)(\ell+1+t)} + \frac{pq\ell}{(2+t)(\ell+2+t)} \\
 &+ \frac{pq\ell}{(1+t)(\ell+1+t)}.
 \end{aligned}$$

Similarly, we have

$$\begin{aligned}
 RDD_{\times}^t(G_2) - RDD_{\times}^t(G) &= p \sum_{x \in H-u-v} \delta(x) \left[\frac{d(x, u) - d(x, v)}{(d(x, u) + 1 + t)(d(x, v) + 1 + t)} \right] \\
 &+ p \sum_{x \in H-u-v} \delta(x) \left[\frac{d(x, u) - d(x, v)}{(d(x, v) + t)(d(x, u) + t)} \right] \\
 &+ \frac{2p\ell(\delta_H(v) - \delta_H(u))}{(1+t)(\ell+1+t)} + \frac{pq\ell}{(2+t)(\ell+2+t)} \\
 &+ \frac{pq\ell}{(1+t)(\ell+1+t)}.
 \end{aligned}$$

If $RDD_{\times}^t(G_1) - RDD_{\times}^t(G) > 0$, then the result follows. Otherwise the inequality is inverse, it immediately follows that

$$\begin{aligned}
 &\sum_{x \in H-u-v} \delta(x) \left[\frac{d(x, u) - d(x, v)}{(d(x, u) + 1 + t)(d(x, v) + 1 + t)} \right] \\
 &+ \sum_{x \in H-u-v} \delta(x) \left[\frac{d(x, u) - d(x, v)}{(d(x, u) + t)(d(x, v) + t)} \right] \\
 &\geq \frac{2\ell(\delta_H(u) - \delta_H(v))}{(1+t)(\ell+1+t)} + \frac{p\ell}{(1+t)(\ell+1+t)} + \frac{p\ell}{(2+t)(\ell+2+t)}.
 \end{aligned}$$

Hence,

$$RDD_{\times}^t(G_2) - RDD_{\times}^t(G) \geq \frac{p\ell(p+q)}{(1+t)(\ell+1+t)} + \frac{p\ell(p+q)}{(2+t)(\ell+2+t)} > 0.$$

This completes the proof. ■

For a unicyclic graph G of order n with girth k , by using transformation $G \Rightarrow \widehat{G}$ in Lemma 2 repeatedly, we can get a unicyclic graph from C_k by adding $n - k$ pendent vertices to the vertices of C_k ; then using transformation $G \Rightarrow G_i$ in Lemma 3 repeatedly, we can get the unicyclic graph $U_{n,k}$.

From Lemma 2.4 and Lemma 3.1, one can easily deduce the following result.

Theorem 4. *Let G be a unicyclic graph of order n with girth k . Then $RDD_{\times}^t(G) \leq RDD_{\times}^t(U_{n,k})$ with equality if and only if G is isomorphic to $U_{n,k}$.*

Theorem 4 shows that $U_{n,k}$ is the unicyclic graph with the maximum reformulated reciprocal product–degree distance among all unicyclic graph of order n and girth k .

4 Relation between RDD_+^t and RDD_\times^t

The well known *first Zagreb index* is defined as [23]

$$M_1(G) = \sum_{v \in V(G)} \delta(v)^2.$$

The *inverse degree* of a graph G with no isolated vertices is

$$R(G) = \sum_{v \in V(G)} \frac{1}{\delta(v)}.$$

The inverse degree first attracted attention through conjectures of the computer program Graffiti [20]. It has been studied by several authors, for example in [8, 19].

In what follows, we discuss the relation between the reciprocal sum–degree distance and the reciprocal product–degree distance. We start with an auxiliary lemma proved by Dragomir in [15] which will be used in later proofs.

Lemma 4. *Let $\vec{x} = (x_1, x_2, \dots, x_N)$ and $\vec{y} = (y_1, y_2, \dots, y_N)$ be sequences of real numbers, $\vec{z} = (z_1, z_2, \dots, z_N)$ and $\vec{w} = (w_1, w_2, \dots, w_N)$ be nonnegative sequences, then*

$$\sum_{i=1}^N w_i \sum_{i=1}^N z_i x_i^2 + \sum_{i=1}^N z_i \sum_{i=1}^N w_i y_i^2 \geq 2 \sum_{i=1}^N z_i x_i \sum_{i=1}^N w_i y_i. \quad (11)$$

In particular, if z_i and w_i are positive, then the equality holds in (11) if and only if $\vec{x} = \vec{y} = \vec{k}$, where $\vec{k} = (k, k, \dots, k)$ is a constant sequence.

Theorem 5. *Let G be a connected graph with n vertices, m edges, maximum degree Δ , minimum degree $\underline{\Delta}$, and forgotten index $F(G)$. Then*

$$2RDD_+^t(G)RDD_\times^t(G) \leq \left[\frac{2m}{(1+t)^2} M_1(G) - \frac{1}{(1+t)^2} F(G) \right] \times \left[\frac{(n-1)\Delta\underline{\Delta}}{\Delta + \underline{\Delta}} + \frac{(n-1)(n-2)\Delta}{4} + (n-1)R(G) \right], \quad (12)$$

with equality if and only if G is isomorphic to K_3 .

Proof. Suppose that each i in Lemma 4 corresponds a vertex pair (v_i, v_j) such that $N = \binom{n}{2}$. Setting $z_i = w_i = \frac{1}{x_i y_i}$ and each x_i is replaced by $\frac{d(v_i, v_j) + t}{\delta(v_i) \delta(v_j)}$ and y_i is replaced by $\frac{d(v_i, v_j) + t}{\delta(v_i) + \delta(v_j)}$, then we get

$$\begin{aligned} \sum_{(v_i, v_j)} \frac{\delta(v_i) \delta(v_j) (\delta(v_i) + \delta(v_j))}{(d(v_i, v_j) + t)^2} \sum_{(v_i, v_j)} \left[\frac{\delta(v_i) + \delta(v_j)}{\delta(v_i) \delta(v_j)} + \frac{\delta(v_i) \delta(v_j)}{\delta(v_i) + \delta(v_j)} \right] \\ \geq 2 \sum_{(v_i, v_j)} \frac{\delta(v_i) + \delta(v_j)}{d(v_i, v_j) + t} \sum_{(v_i, v_j)} \frac{\delta(v_i) \delta(v_j)}{d(v_i, v_j) + t}. \end{aligned} \tag{13}$$

In order to accomplish the proof, it is sufficient to find respectively the upper bound of

$$\zeta_1(v_i, v_j) = \sum_{(v_i, v_j)} \left[\frac{\delta(v_i) + \delta(v_j)}{\delta(v_i) \delta(v_j)} + \frac{\delta(v_i) \delta(v_j)}{\delta(v_i) + \delta(v_j)} \right].$$

and

$$\zeta_2(v_i, v_j) = \sum_{(v_i, v_j)} \frac{\delta(v_i) \delta(v_j) (\delta(v_i) + \delta(v_j))}{(d(v_i, v_j) + t)^2}.$$

Note that $\frac{2}{\Delta} \leq \frac{1}{\delta(v_i)} + \frac{1}{\delta(v_j)} \leq \frac{2}{\underline{\Delta}}$, it immediately follows that $\frac{\delta(v_i) \delta(v_j)}{\delta(v_i) + \delta(v_j)} \leq \frac{\Delta}{2}$. Again since $\frac{1}{\Delta} + \frac{1}{\underline{\Delta}} \leq \frac{1}{\delta(v_i)} + \frac{1}{\underline{\Delta}}$, we have $\frac{\delta(v_i) \underline{\Delta}}{\delta(v_i) + \underline{\Delta}} \leq \frac{\Delta \underline{\Delta}}{\Delta + \underline{\Delta}}$. Suppose that v_n is the minimum degree vertex of degree $\underline{\Delta}$. Using the above results, we have

$$\begin{aligned} \sum_{(v_i, v_j)} \frac{\delta(v_i) \delta(v_j)}{\delta(v_i) + \delta(v_j)} &= \sum_{(v_i, v_n)} \frac{\delta(v_i) \underline{\Delta}}{\delta(v_i) + \underline{\Delta}} + \sum_{\substack{(v_i, v_j) \\ v_j \neq v_n}} \frac{\delta(v_i) \delta(v_j)}{\delta(v_i) + \delta(v_j)} \\ &\leq \frac{(n-1) \Delta \underline{\Delta}}{\Delta + \underline{\Delta}} + \left[\frac{n(n-1)}{2} - (n-1) \right] \frac{\Delta}{2} \\ &= \frac{(n-1) \Delta \underline{\Delta}}{\Delta + \underline{\Delta}} + \frac{(n-1)(n-2) \Delta}{4}. \end{aligned} \tag{14}$$

By simple calculations, we get

$$\sum_{(v_i, v_j)} \frac{\delta(v_i) + \delta(v_j)}{\delta(v_i) \delta(v_j)} = \sum_{(v_i, v_j)} \left[\frac{1}{\delta(v_i)} + \frac{1}{\delta(v_j)} \right] = \sum_{v_i \in V(G)} \frac{n-1}{\delta(v_i)} = (n-1)R(G). \tag{15}$$

Inequalities (14) and (15) yield

$$\begin{aligned} \zeta_1(v_i, v_j) &= \sum_{(v_i, v_j)} \left[\frac{\delta(v_i) \delta(v_j)}{\delta(v_i) + \delta(v_j)} + \frac{\delta(v_i) + \delta(v_j)}{\delta(v_i) \delta(v_j)} \right] \\ &\leq \frac{(n-1) \Delta \underline{\Delta}}{\Delta + \underline{\Delta}} + \frac{(n-1)(n-2) \Delta}{4} + (n-1)R(G). \end{aligned} \tag{16}$$

Note that by $\sum_{v_i \in V(G)} \delta(v_i) = 2m$ and $d(v_i, v_j) \geq 1$, it holds that

$$\begin{aligned} \zeta_2(v_i, v_j) &= \sum_{(v_i, v_j)} \frac{\delta(v_i)\delta(v_j)(\delta(v_i) + \delta(v_j))}{(d(v_i, v_j) + t)^2} \leq \sum_{(v_i, v_j)} \frac{\delta(v_i)\delta(v_j)(\delta(v_i) + \delta(v_j))}{(1 + t)^2} \\ &= \sum_{v_i \in V(G)} \frac{\delta^2(v_i)(2m - \delta(v_i))}{(1 + t)^2} = \frac{2m}{(1 + t)^2} M_1(G) - \frac{1}{(1 + t)^2} F(G). \end{aligned} \tag{17}$$

Using (16) and (17), we get the required result in (12). The first part of the proof is done.

Now we assume that the equality holds in (12). From equality in (13), by Lemma 4, we get

$$\frac{d(v_i, v_j) + t}{\delta(v_i)\delta(v_j)} = \frac{d(v_i, v_k) + t}{\delta(v_i)\delta(v_k)} = \frac{d(v_i, v_j) + t}{\delta(v_i) + \delta(v_j)} = \frac{d(v_i, v_k) + t}{\delta(v_i) + \delta(v_k)}$$

and $d(v_i, v_j) = d(v_i, v_k)$ holds for any vertices v_i, v_j and v_k of graph G . This implies that $\delta(v_i) = \delta(v_j) = 2$ and $D(G) = 1$. Hence $G \cong K_3$. Conversely, one can easily see that the equality holds in (12) for K_3 . ■

The following is an immediate consequence of Theorem 5.

Corollary 5. *Let G be a connected graph with n vertices, m edges, maximum degree Δ , minimum degree $\underline{\Delta}$ and p pendent vertices, then*

$$\begin{aligned} 2RDD_+^t(G)RDD_\times^t(G) &\leq \left[\frac{2m - \underline{\Delta}}{(1 + t)^2} M_1(G) + \frac{\underline{\Delta} - 1}{(1 + t)^2} p \right] \\ &\times \left[\frac{(n - 1)\underline{\Delta}\underline{\Delta}}{\underline{\Delta} + \underline{\Delta}} + \frac{(n - 1)(n - 2)\underline{\Delta}}{4} + (n - 1)R(G) \right], \end{aligned} \tag{18}$$

with equality if and only if G is isomorphic to K_3 .

Proof. Since p is the number of pendent vertices in G , it follows that

$$\begin{aligned} \sum_{v_i \in V(G)} \delta(v_i)^3 &= p + \sum_{v_i \in V(G), \delta(v_i) \neq 1} \delta(v_i)^3 \\ &\geq p + \underline{\Delta} \sum_{v_i \in V(G), \delta(v_i) \neq 1} \delta(v_i)^2 = p + \underline{\Delta}(M_1(G) - p). \end{aligned} \tag{19}$$

Applying inequality (19) to $\zeta_2(v_i, v_j)$, yields

$$\begin{aligned} \zeta_2(v_i, v_j) &\leq \sum_{(v_i, v_j)} \frac{\delta(v_i)\delta(v_j)(\delta(v_i) + \delta(v_j))}{(1 + t)^2} = \sum_{v_i \in V(G)} \frac{\delta(v_i)^2(2m - \delta(v_i))}{(1 + t)^2} \\ &\leq \frac{2m - \underline{\Delta}}{(1 + t)^2} M_1(G) + \frac{\underline{\Delta} - 1}{(1 + t)^2} p. \end{aligned}$$

We get the required result (18). Moreover, the equality holds in (18) if and only if G is isomorphic to K_3 . ■

Lemma 6. (Radon’s inequality) *For real numbers $a_1, a_2, \dots, a_N \geq 0, b_1, b_2, \dots, b_N > 0$, and $p > 0$, the following inequality holds:*

$$\sum_{i=1}^N \frac{a_i^{p+1}}{b_i^p} \geq \frac{\left(\sum_{i=1}^N a_i\right)^{p+1}}{\left(\sum_{i=1}^N b_i\right)^p}.$$

We now give another relation between the reciprocal sum–degree distance and reciprocal product–degree of graphs.

Theorem 6. *Let G be a connected graph with n vertices, m edges, maximum degree Δ and minimum degree $\underline{\Delta}$, then*

$$\frac{(RDD_+^t(G))^2}{RDD_\times^t(G)} \leq \frac{(\Delta + \underline{\Delta})^2}{\Delta \underline{\Delta}} H_t(G).$$

with equality if and only if G is a regular graph.

Proof. Assume that each i in Lemma 6 corresponds a vertex (v_i, v_j) with $N = \binom{n}{2}$ and $p = 1$. Setting each a_i is replaced by $\frac{\delta(v_i)+\delta(v_j)}{d(v_i, v_j)+t}$ and b_i is replaced by $\frac{\delta(v_i)\delta(v_j)}{d(v_i, v_j)+t}$, it follows that

$$\frac{\left(\sum_{(v_i, v_j)} \frac{\delta(v_i)+\delta(v_j)}{d(v_i, v_j)+t}\right)^2}{\sum_{(v_i, v_j)} \frac{\delta(v_i)\delta(v_j)}{d(v_i, v_j)+t}} \leq \sum_{(v_i, v_j)} \frac{\left(\frac{\delta(v_i)+\delta(v_j)}{d(v_i, v_j)+t}\right)^2}{\frac{\delta(v_i)\delta(v_j)}{d(v_i, v_j)+t}},$$

which is equivalent to

$$\frac{(RDD_+^t(G))^2}{RDD_\times^t(G)} \leq \sum_{(v_i, v_j)} \left(\sqrt{\frac{\delta(v_i)}{\delta(v_j)}} + \sqrt{\frac{\delta(v_j)}{\delta(v_i)}}\right)^2 \frac{1}{d(v_i, v_j) + t}.$$

It has been proved in [9] that

$$\left(\sqrt{\frac{\delta(v_i)}{\delta(v_j)}} + \sqrt{\frac{\delta(v_j)}{\delta(v_i)}}\right)^2 \leq \frac{(\Delta + \underline{\Delta})^2}{\Delta \underline{\Delta}}.$$

Moreover, the equality holds if and only if G is a regular graph or G is a bipartite semiregular graph. Hence, we obtain

$$\frac{(RDD_+^t(G))^2}{RDD_\times^t(G)} \leq \sum_{(v_i, v_j)} \frac{(\Delta + \underline{\Delta})^2}{\Delta \underline{\Delta}} \frac{1}{d(v_i, v_j) + t} = \frac{(\Delta + \underline{\Delta})^2}{\Delta \underline{\Delta}} H_t(G).$$

The equality holds if and only if G is a regular graph. ■

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