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Relation with Reformulated Reciprocal Degree Distance and other Graph Parameters

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Abstract The reciprocal degree distance (RDD), defined for a connected graph G as vertex degree-weighted sum of the reciprocal distances, that is $RDD(G) = \sum\limits_{u,v \in V(G)} \frac{d_G(u)+d_G(v)}{d_G(u,v)}$ .The reformulated reciprocal degree distance of Graph $\overline{R}_t(G)$, is defined as $\overline{R}_t(G) = \sum\limits_{u,v \in V(G)} \frac{d_G(u)+d_G(v)}{d_G(u,v)+t}$, where t is any real number. In this paper, we investigate the relation between the reformulated reciprocal degree distance and other graph parameters.

1 Introduction

All the graphs considered in this paper are simple and connected. For vertices $u, v \in V(G)$,the distance between u and v in G,denoted by $d_G(u, v)$ include the depth eccentricity diameter,is the length of a shortest(u, v)-path in G and $d_G(v)$ is the degree of a vertex$v \in V(G)$.A single number that can be used to characterize some property of the graph of a molecule is called a *topological index*.Topological index is a graph theoretical 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.The interest in topological in-dices is mainly related to their use in non-empirical quantitative structure-property relationships and quantitative structural-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 Wiener as the sum of distance over all unordered vertex pairs in G, namely, $W(G) = \frac{1}{2} \sum\limits_{u,v \in V(G)} d_G(u, v)$.This definition can be further generalized in the following way: $W_\lambda(G) = \frac{1}{2} \sum\limits_{u,v \in V(G)} d_G(u, v)^\lambda$, where $d_G(u, v)^\lambda = d_G^\lambda(u, v)and\lambda$ is a real number [4]. Another distance based graph invariant, defined in a fully analogous manner to winner index, is the*Harary index,* which is equal to the sum of the the reciprocal distances overall unordered vertex pairs in G, that is, $H(G) = \frac{1}{2} \sum\limits_{u,v \in V(G)} \frac{1}{d_G(u,v)}$.Dobrynin and Kochetova [2] and Gutman [3] independently proposed a vertex-degree-weighted version of Wiener index called *degree distance*, which is defined for a connected graph G as $DD(G) = \frac{1}{2} \sum\limits_{u,v \in V(G)} (d_G(u) + d_G(v))d_G(u, v)$. The *additively weighted Harary index*(H_A) or *reciprocal degree distance*(RDD) is defined in [1] as $H_A(G) = RDD(G) = \frac{1}{2} \sum\limits_{u,v \in V(G)} \frac{(d_G(u)+d_G(v))}{d_G(u,v)}$. Hua and Zhang [5] have obtained lower and upper bounds for the reciprocal degree distance of graph in terms of other graph invariants.The chemical applications and mathematical properties of the reciprocal degree distance are well studied in [1, 6, 9].Similarly consider the generalized version of *Harary index*, namely the t-Harary index, which is defined as $\overline{H}_t(G) = \frac{1}{2} \sum\limits_{u,v \in V(G)} \frac{1}{d_G(u,v)+t}$,where t is any real number.

Recently, Li et al. introduced a vertex-degree-weighted version of t-Harary index called reformulated reciprocal degree distance, which is defined for a connected graph G as The *reformulated reciprocal degree distance of graph* , denoted by $\overline{R}_t(G)$ is defined as $\overline{R}_t(G) =$

$\frac{1}{2}\sum\limits_{u,v\in V(G)}\frac{d_G(u)+d_G(v)}{d_G(u,v)+t}$, where t is any real number.In this paper we investigate the reformulated reciprocal degree distance with other graph parameters and then determine the extremal values of this new invariant for general graphs.

2 Bounds Related to other graph parameters

In this section, we compute the bounds for reformulated reciprocal degree distance of a connected graph in terms of other graph parameters. The minimum and maximum degree of the graph G are denoted by $\delta(G)$ and $\Delta(G)$, respectively. The first Zagreb index of G denoted by $M_1(G)$ is defined as $M_1(G) = \sum\limits_{u\in V(G)}(d_G(u))^2 = \sum\limits_{uv\in E(G)}(d_G(u)+d_G(v))$. Similarly, the first Zagreb coindex of G is defined as $\overline{M_1}(G) = \sum\limits_{uv\notin E(G)}(d_G(u)+d_G(v))$.

Theorem 2.1. *Let G be a nontrivial connected graph.Then $\overline{R}_t(G) \leq DD(G)$, with equality if and only if $G \cong K_n$.*

Proof. For any two vertices $u$and v in G,we have $\frac{1}{d_G(u,v)+t} \leq \frac{1}{d_G(u,v)} \leq d_G(u,v)$ with equality if and only if $d_G(u,v) = 1\ \ and\ t = 0$.we have

$$\overline{R}_t(G) = \sum_{u,v\in V(G)}\frac{d_G(u)+d_G(v)}{d_G(u,v)+t} \leq \sum_{u,v\in V(G)}(d_G(u)+d_G(v))d_G(u,v) = DD(G).$$

Where $DD(G)$ is the degree distance of G. Equality holds if and if $d_G(u,v) = 1$ and $t = 0$ that is if and only if $G \cong K_n$ and $t = 0$.

Theorem 2.2. *Let G be a nontrivial connected graph.Then $\overline{R}_t(G) \leq M_1(G) + \overline{M}_1(G)$,with equality if $G \cong K$.*

Proof. For any vertex x in G,we have $\overline{R}_t(G) \leq \sum_{\{u,v\}\subseteq V(G)}\frac{d_G(u)+d_G(v)}{d_G(u,v)+t}$, where $t \geq 0$.
One can see that$\frac{1}{d_G(u,v)+t} \leq 1$ with equality if and only if $d_G(u,v) = 1$ and $t = 0$. Hence

$$\begin{aligned}
\overline{R}_t(G) &\leq \sum_{\{u,v\}\subseteq V(G)}(d_G(u)+d_G(v)). \\
&= \sum_{uv\in E(G)}(d_G(u)+d_G(v)) + \sum_{uv\notin E(G)}(d_G(u)+d_G(v)) \\
&= \sum_{x\in V(G)}(d_G(x))^2 + \overline{M}_1(G) \\
&= M_1(G) + \overline{M}_1(G).
\end{aligned}$$

Thus we have $\overline{R}_t(G) \leq M_1(G) + \overline{M}_1(G)$ with equality if and only if for any two vertices u and v in G,$d_G(u,v) = 1$, i.e $G \cong K_n$ and $t = 0$.

Theorem 2.3. *Let G be a connected graph.Then $2\delta(G)H_t(G) \leq \overline{R}_t(G) \leq 2\Delta(G)H_t(G)$,with either equality if and only if G is a regular graph*

Proof. For any vertex x in G,we have $\delta(G) \leq d_G(x) \leq \Delta(G)$. Hence

$$2\delta(G)\sum_{\{u,v\}\subseteq V(G)}\frac{1}{d_G(u,v)+t} \leq \overline{R}_t(G) \leq 2\Delta(G)\sum_{\{u,v\}\subseteq V(G)}\frac{1}{d_G(u,v)+t}.$$

This implies,

$$2\delta(G)H_t(G) \leq \overline{R}_t(G) \leq 2\Delta(G)H_t(G).$$

Theorem 2.4. *Let G be a connected graph. Then* $\overline{R}_t(G) \geq \frac{(M_1(G)+\overline{M_1}(G))^2}{DD(G)}$, $t \geq 0$ *with equality if and only if* $t = 0$ *and* $G \cong K_n$.

Proof. By the definition of degree distance and reformulated degree distance

$$DD(G)\overline{R}_t(G) = \Bigg(\sum_{\{u,v\} \subseteq V(G)} \Big(d_G(u) + d_G(v) \Big) d_G(u,v) \Bigg) \Bigg(\sum_{\{u,v\} \subseteq V(G)} \frac{d_G(u) + d_G(v)}{d_G(u,v) + t} \Bigg)$$

$$\begin{aligned} DD(G)\overline{R}_t(G) &\geq \Bigg(\sum_{u,v \in V(G)} (d_G(u) + d_G(v)) \Bigg)^2 \\ &= \Bigg(\sum_{\{u,v\} \subseteq V(G)} (d_G(u) + d_G(v)) + \sum_{uv \notin E(G)} (d_G(u) + d_G(v)) \Bigg)^2 \\ &= (M_1(G) + \overline{M_1}(G))^2. \end{aligned}$$

Equality holds if and only if $d_G(u,v)$ is constant in G and $t = 0$.
This implies $G \cong K_n$ and t=0.

Definition of the reformulated reciprocal degree distance is equivalent to

$$\overline{R}_t(G) = \sum_{u \in V(G)} d_G(u) \widetilde{D}_G(u),$$

where

$$\widetilde{D}_G(u) = \sum_{v \in V(G)} \frac{1}{d_G(u,v) + t}.$$

Theorem 2.5. *Let G be a connected graph of order $n \geq 2$ and size $m \geq 1$. Then* $\frac{2(n-1)m}{d+t} + \frac{(d-t)M_1(G)}{d+t} \leq \overline{R}_t(G) \leq \frac{1}{2+t} 2(n-1)m + (1+t)M_1(G)$, $t \geq 0$ *with equality if and only if* $t = 0$ *and* $G \cong K_n$.

Proof. With either equality if and only if $d(G) \leq 2$, where d(G)-diameter of G.

$$\begin{aligned} \widetilde{D}_G(x) &= d_G(x) + \sum_{y \in V(G) \setminus N_G(x)} \frac{1}{d_G(x,y) + t} \\ &\leq d_G(x) + \frac{n - d_G(x) - 1}{2 + t} \\ &\leq \frac{n + (1+t)d_G(x) - 1}{2 + t} \\ &= \frac{(n-1) + (1+t)d_G(x)}{2 + t}. \end{aligned}$$

Equality is attained if and only if $e(x) \leq 2$,where $e(x)$-eccentricity of x in G. From above inequality it follows immediately that

$$\begin{aligned}
\overline{R}_t(G) &= \sum_{u\in V(G)} d_G(u)\widetilde{D}_G(u) \\
&\leq \sum_{x\in V(G)} d_G(x)\widetilde{D}_G(x) \\
&\leq \sum_{x\in V(G)} d_G(x)\frac{(n-1)+(1+t)d_G(x)}{2+t}. \\
&= \frac{(n-1)}{2+t}\sum_{x\in V(G)} d_G(x) + \frac{(1+t)}{2+t}\sum_{x\in V(G)} (d_G(x))^2 \\
&= \frac{(n-1)}{2}m2+t+\frac{(1+t)}{2+t}\sum_{x\in V(G)} (d_G(x))^2 \\
&= \frac{1}{2+t}\left[\frac{(n-1)}{2}m+(1+t)\sum_{x\in V(G)} (d_G(x))^2\right]
\end{aligned}$$

Equality is attained if and only if $e(x) \leq 2$,$t \geq 0$. Hence,

$$\overline{R}_t(G) \leq \frac{1}{2+t}\left[(n-1)2m+(1+t)\sum_{x\in V(G)} (d_G(x))^2\right]$$

with equality if and if the diameter of G is at most 2,as desired.
Now taking left-hand side inequality.For each vertex x in G we have

$$\begin{aligned}
\widetilde{D}_G(x) &= d_G(x) + \sum_{y\in V(G)\setminus N_G(x)} \frac{1}{d_G(x,y)+t} \\
&\geq d_G(x) + \frac{n-d_G(x)-1}{d+2} \\
&= \frac{(n-1)+(d-t)d_G(x)}{d+2}.
\end{aligned}$$

Therefore

$$\begin{aligned}
\overline{R}_t(G) &\geq \sum_{x\in V(G)} d_G(x)\widetilde{D}_G(x) \\
&= \sum_{x\in V(G)} d_G(x)\left[\frac{(n-1)+(d-t)d_G(x)}{d+t}\right]. \\
&= \frac{(n-1)}{d+t}\sum_{x\in V(G)} d_G(x) + \frac{(d-t)}{d+t}\sum_{x\in V(G)} (d_G(x))^2 \\
&= \frac{2(n-1)m}{d+t} + \frac{(d-t)M_1(G)}{d+t}
\end{aligned}$$

where the equality is attained if and if the diameter of G is $\leq$ 2,as desired. A cactus is a connected graph each of whose blocks is either a cycle or an edge. If a cactus has no cycles, then it is just a tree, and if it has exactly a cycle , then it is a unicyclic graph. For $0 \leq k \leq \frac{n-1}{2}$, we let G_n^k be an n-vertex star by adding k-independent edges among $n-1$ pendent vertices.In the following we shall give a sharp upper bound for $\overline{R}_t(G)$ of k- cycle cactus[10].

Lemma 2.6. *Let G be an n vertex k-cycle cactus with$0 \leq k \leq \frac{n-1}{2}$.Then $M_1(G) \leq n^2 - n + 6k$ with equality if and only if $G \cong K_n$.*

Theorem 2.7. *Let G be an n-vertex k-cycle cactus with $0 \leq k \leq \frac{n-1}{2}$. Then $\overline{R}_t(G) \leq \frac{(n-1)(n+k-1)+(1+t)(n^2-n+6k)}{2+t}$,with equality if and only $G \cong K_n$ and $t = 0$.*

Proof. Note that G has $n + k - 1$ edges. By Theorem 2.5 and Lemma 2.6, we have

$$\begin{aligned}
\overline{R}_t(G) &\leq \frac{1}{2+t}\Big[2(n-1)(n+k-1) + (1+t)M_1(G)\Big] \\
&\leq \frac{1}{2+t}\Big[2(n-1)(n+k-1) + (1+t)M_1(G_n^2)\Big] \\
&= \frac{1}{2+t}\Big[2(n-1)(n+k-1) + (1+t)(n^2-n+6k)\Big] \\
&= \frac{1}{2+t}\Big[2(n-1)(n+k-1) + (1+t)(n^2-n+6k)\Big]
\end{aligned}$$

The above first equality holds if and if the diameter of G is 2 and $t = 0$ and the second one holds if and only if$G \cong K_n$and $t = 0$. Note that G_n^k has diameter 2.Thus,$\overline{R}_t(G) \leq \frac{(n-1)(n+k-1)+(1+t)(n^2-n+6k)}{2+t}$with equality if and only if $G \cong G_n^K$ and $t = 0$. By theorem 2.7, we immediately have following results for $\overline{R}_t(G)$ of trees and unicyclic graphs,respectively.
Corollary 1. Let T be a tree on $n \geq 2$ vertices.Then
$\overline{R}_t(G) \leq \frac{n-1}{2+t}\Big[(n-1) + n(1+t)\Big]$
with equality if and only if $T \cong S_n$ and $t = 0$.
Corollary 2. Let G be a uni cyclic graph on $n \geq 3$ vertices.Then
$\overline{R}_t(G) \leq \frac{1}{2+t}\Big[n(n-1) + (1+t)(n^2-n+6)\Big]$,
with equality if and only if $G \cong G_n^1$ and $t = 0$. Let K_n^p denote the graph obtained by attaching p pendent edges to a vertex of K_{n-p}.We first prove the following result.

Lemma 2.8. *Let G be an n-vertex connected graph with p pendent vertices. Then*
$M_1(G) \leq n^3 - (3p-1)n^2 + (3p^2+6p+1)n - p^3 - 3p^2 - 2p - 1$

with equality if and only if $G \cong K_n^p$ and $t = 0$.
Proof. Suppose that G_{max} is a graph chosen among all connected graphs with n vertices and p pendent vertices such that it has the maximum first Zagreb index. Let $D(G_{max}) = \{x_1, x_2, \ldots, x_n\}$ denote the degree sequence of G_{max}. If we label all pendent vertices of G_{max} as $v_1, \ldots, v_p$, then $G[V(G_{max}) \setminus \{v_1, \ldots, v_p\}]$, the sub-graph of G_{max} induced by vertices in $V(G_{max}) \setminus \{v_1, \ldots, v_p\}$ must be a clique in G_{max}, for otherwise, we can obtain a new graph with a strictly larger first Zagreb index than that of G_{max} by adding edges into G_{max}.Note that the degree sequence $D(K_n^p) = \underbrace{\{n-1, n-p-1, \ldots, n-p-1\}}_{n-p-1}, \underbrace{1, \ldots, 1}_{p}$.If $G_{max} \ncong K_n^p$,then there must exist a pair (x_i, x_j), in G_{max} with $n - p \leq x_i \leq x_j \leq n - 2$. We construct a new n-vertex and p-pendent vertex connected graph G' by replacing the pair (x_i, x_j) in G_{max} by the pair $(x_i - 1, x_j + 1)$. It is easy to obtain that $M_1(G') > M_1(G_{max})$, a contradiction to our choice of G_{max}.
Then $G_{max} \cong K_n^p$.
Also,$M_1(K_n^p) = (n-1)^2 + p + (n-p-1)^3 = n^3 - (3p-1)n^2 + (3p^2+6p+1)n - p^3 - 3p^2 - 2p - 1.$

Theorem 2.9. *Let G be an n-vertex connected graph with $p$pendent vertices. Then*
$\overline{R}_t(G) \leq \frac{1}{2+t}\left[(n-1)\frac{[(n-1)^2+3p-n]}{2}+(1+t)(n^3-(3p-1)n^2+(3p^2+6p+1)n-p^3-3p^2-2p-1\right]$
with equality if $G \cong K_n^p$ and $t=0$.

Proof. Let G^* be a connected graph with n vertices and p-pendent vertices $v_1,\ldots,v_p$,satisfies that $G[V(G_{max})/\{v_1,\ldots,v_p\}]$,the sub graph of induced by vertices in $V(G)/\{v_1,\ldots,v_p\}$, is a clique inG^*We need only to consider the upper bound for $\overline{R}_t(G)$ of G^*.It is obvious that G^* has p+$\binom{n-p}{2}$=$p+\frac{(n-p)(n-p-1)}{2}$ edges. By Theorem 2.5 and Lemma 2.8, we have

$$\overline{R}_t(G) \leq \frac{1}{2+t}\Big[(n-1)2m + M_1(G^*)\Big]$$
$$\overline{R}_t(G) = \frac{1}{2+t}\left[(n-1)[(n-p)^2+3p-n] + M_1(G^*)\right]$$
$$\overline{R}_t(G) \leq \frac{1}{2+t}\left[(n-1)[(n-p)^2+3p-n] + M_1(K_n^p)\right]$$
$$\overline{R}_t(G) = \frac{1}{2+t}\Big[(n-1)[(n-p)^2+3p-n] + (1+t)n^3 - (3p-1)n^2 + (3p^2+6p+1)n - p^3 - 3p^2 - 2p - 1\Big].$$

The first equality holds if and only if the diameter ofG^* is at most 2 and the second one holds if and only if $G \cong K_n^p$ and $t=0$. Note that K_n^p has diameter 2. Hence

$$\overline{R}_t(G) = \frac{1}{2+t}\Big[(n-1)[(n-p)^2+3p-n] + (1+t)n^3 - (3p-1)n^2 + (3p^2+6p+1)n - p^3 - 3p^2 - 2p - 1\Big]$$

. With equality if and only if $G \cong K_n^p$ and $t=0$. This completes the proof.

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