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Reciprocal Product–Degree Distance of Graphs

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Abstract. We investigate a new graph invariant named reciprocal product–degree distance, defined as:

$$RDD_* = \sum_{\substack{\{u,v\}\subseteq V(G)\\ u\neq v}} \frac{\deg(u)\cdot\deg(v)}{\mathrm{dist}(u,v)}$$

where $\deg(v)$ is the degree of the vertex v, and $\mathrm{dist}(u,v)$ is the distance between the vertices u and v in the underlying graph. RDD_* is a product–degree modification of the Harary index. We determine the connected graph of given order with maximum RDD_*-value, and establish lower and upper bounds for RDD_*. Also a Nordhaus–Gaddum–type relation for RDD_* is obtained.

1. Introduction

Throughout this paper, we consider finite undirected simple connected graphs. Let $G = (V, E)$ be such a graph. We denote its order and size with $|V|$ and $|E|$ if no ambiguity can arise. The *degree* of a vertex $u \in V$ is the number of edges incident to u, denoted by $\deg_G(u)$. The maximum and minimum vertex degree in the graph G will be denoted by $\Delta(G)$ and $\delta(G)$, respectively. The *distance* between two vertices u and v is the length of a shortest path connecting them in G, denoted by $\mathrm{dist}_G(u,v)$. The maximum value of such numbers, $\mathrm{diam}(G)$, is said to be the *diameter* of G.

The *complement* of G, denoted by $\overline{G}$, is the graph with vertex set $V(G)$, in which two distinct vertices are adjacent if and only if they are not adjacent in G. Other terminology and notations needed will be introduced as it naturally occurs, and we use [4] for those not defined here.

The motivation for studying the quantity that we intend to call *reciprocal product–degree distance* of a graph, comes from the following observation. The sum of distances between all pairs of vertices in a graph G, namely

$$W = W(G) = \sum_{\{u,v\}\subseteq V(G)} \mathrm{dist}_G(u,v) \tag{1}$$

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was first time introduced by Wiener more that 60 years ago [31]. Initially, the Wiener index $W(G)$ was considered as a molecular–structure descriptor used in chemical applications, but soon it attracted the interest of "pure" mathematicians [11, 12]; for details and additional references see the reviews [7, 35] and the recent papers [22, 23, 34].

Eventually, a number of modifications of the Wiener index were proposed, which we present in the following table:

W	DD_+	DD_*
H	RDD_+	RDD_*?

Table 1. A family of distance– and degree–based graph invariants.

In Table 1, W is the ordinary Wiener index, Eq. (1), whereas

$$DD_+ = DD_+(G) = \sum_{\{u,v\}\subseteq V(G)} \Big[\deg_G(u) + \deg_G(v)\Big]\mathrm{dist}_G(u,v) \tag{2}$$

$$DD_* = DD_*(G) = \sum_{\{u,v\}\subseteq V(G)} \Big[\deg_G(u) \cdot \deg_G(v)\Big]\mathrm{dist}_G(u,v) \tag{3}$$

$$H = H(G) = \sum_{\substack{\{u,v\}\subseteq V(G)\\ u\neq v}} \frac{1}{\mathrm{dist}_G(u,v)} \tag{4}$$

$$RDD_+ = RDD_+(G) = \sum_{\substack{\{u,v\}\subseteq V(G)\\ u\neq v}} \frac{\deg_G(u) + \deg_G(v)}{\mathrm{dist}_G(u,v)}\,. \tag{5}$$

The graph invariants defined via Eqs. (2)–(4) have all been much studied in the past. The invariant DD_+ was first time introduced by Dobrynin and Kochetova [8] and named *(sum)–degree distance*. Later the same quantity was examined under the name "Schulz index" [14]. For mathematical research on degree distance see [1, 6, 10, 19, 29] and the references cited therein. A remarkable property of DD_+ is that in the case of trees of order n, the identity $DD_+ = 4W - n(n-1)$ holds [20].

In [33] it was shown that also the multiplicative variant of the degree distance, namely DD_*, Eq. (3), obeys an analogous relation: $DD_* = 4W - (2n-1)(n-1)$. This latter quantity is sometimes referred to as the "Gutman index" (see [2, 13, 21, 25, 26] and the references quoted therein), but here we call it *product–degree distance*.

The greatest contributions to the Wiener index, Eq. (1), come from most distant vertex pairs. Because in many applications of graph invariants it is preferred that the contribution of vertex pairs diminishes with distance, the Wiener index was modified according to Eq. (4). This distance–based graph invariant is called *Harary index* and was introduced in the 1990s by Plavšić et al. [28]. It also was subject of numerous mathematical studies (see [5, 17, 30, 32, 33] and the references cited therein).

Recently, Hua and Zhang [18] introduced and examined the *reciprocal sum–degree distance* RDD_+, which is the first degree–distance–type modification of the Harary index, given by Eq. (5).

The graph invariants, defined via Eqs. (1)–(5), can be arranged as in Table 1. From this Table it is immediately seen that one more such invariants is missing. This is the *reciprocal product–degree distance*, defined as

$$RDD_* = RDD_*(G) = \sum_{\substack{\{u,v\}\subseteq V(G)\\ u\neq v}} \frac{\deg_G(u) \cdot \deg_G(v)}{\mathrm{dist}_G(u,v)}\,. \tag{6}$$

Evidently, the reciprocal product–degree distance is related to the Harary index in the same way as the product–degree distance is related to the Wiener index, cf. Table 1. To our best knowledge, this new

invariant has not been studied so far. Therefore, in this paper we determine some of its basic properties, including those quite elementary.

First we focus our attention to the extremal properties of reciprocal product–degree distance and in Section 2 characterize the connected graphs with maximum RDD_*. In Section 3, we establish lower and upper bounds for RDD_* in terms of other graph invariants, including DD_*, the second Zagreb index, the second Zagreb co-index, Harary index, matching number, independence number and vertex-connectivity. In Section 4, a Nordhaus–Gaddum–type inequality for RDD_* is presented.

In what follows, for the sake of simplicity, instead of $\sum_{\substack{\{u,v\}\subseteq V(G)\\ u\neq v}}$ we shall write $\sum_{\{u,v\}\subseteq V(G)}$, always assuming that $u \neq v$.

2. Connected Graphs with Maximum RDD_*-Value

Let $G - e$ denote the graph formed from G by deleting an edge $e \in E(G)$, and $G + e$ denote the graph obtained from G by adding to it an edge $e \notin E(G)$.

A *cut-edge* is an edge in a graph whose deletion will increase the number of components.

Lemma 1. Let G be a connected graph of order at least three. The following holds:

(**a**) If G is not isomorphic to K_n, then $RDD_*(G) < RDD_*(G + e)$ for any $e \in E(\overline{G})$.

(**b**) If G has an edge e not being a cut-edge, then $RDD_*(G) > RDD_*(G - e)$.

Proof. Suppose that G is not the complete graph. Then G must possess a pair of vertices u and v such that $uv \in E(\overline{G})$. It is obvious that $\mathrm{dist}_G(u, v) \geq \mathrm{dist}_{G+uv}(u, v)$ and $\mathrm{dist}_G(x, y) \geq \mathrm{dist}_{G+uv}(x, y)$ for any pair of vertices $x, y \in V(G)$. In addition, $\deg_G(w) \leq \deg_{G+uv}(w)$ for any vertex $w \in V(G)$. By the definition of reciprocal product-degree distance, we have $RDD_*(G) < RDD_*(G + e)$. This completes the proof of (**a**).

If e is not a cut edge, then $G - e$ is connected and not isomorphic to the complete graph. Thus by (**a**), $RDD_*(G - e) < RDD_*((G - e) + e) = RDD_*(G)$, as desired. □

By means of Lemma 1, we can characterize the connected graphs with maximum RDD_*-value. More precisely, we arrive at the following result.

Theorem 1. Among all connected graphs of order n, the complete graph K_n attains the maximum RDD_*-value $\frac{n(n-1)^3}{2}$.

Proof. If G is not the complete graph, then we can repeatedly add edges into G until we obtain K_n. By Lemma 1, $RDD_*(G) < RDD_*(K_n)$, with equality if and only if $G \cong K_n$. □

3. Relation with Other Graph Parameters

In this section, we present various bounds for the reciprocal product–degree distance in terms of other graph parameters.

3.1. Relation with other topological indices

Theorem 2. Let G be a connected graph of order n. Then $RDD_*(G) \leq DD_*(G)$ with equality if and only if $G \cong K_n$.

Proof. Because $1/\mathrm{dist}_G(u,v) \le \mathrm{dist}_G(u,v)$ for any pair of vertices u, v of G,

$$RDD_*(G) \le \sum_{\{u,v\}\subseteq V(G)} [\deg_G(u)\ \deg_G(v)]\mathrm{dist}_G(u,v) = DD_*(G)\ .$$

Thus $RDD_*(G) \le DD_*(G)$, with equality if and only if $\mathrm{dist}_G = 1$ for any pair of vertices u and v in G, or equivalently, $G \cong K_n$. □

The second Zagreb index and second Zagreb co-index are, respectively, defined as [9, 16]:

$$M_2(G) = \sum_{uv\in E(G)} [\deg_G(u)\ \deg_G(v)] \qquad \text{and} \qquad \overline{M}_2(G) = \sum_{uv\in E(\overline{G})} [\deg_G(u)\ \deg_G(v)]\ .$$

Theorem 3. Let G be a connected graph of order n. Then

$$RDD_*(G) \ge \frac{[M_2(G) + \overline{M}_2(G)]^2}{DD_*(G)}$$

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

Proof. By the definition of reciprocal product–degree distance, and using the Cauchy–Schwarz inequality, we get

$$\begin{aligned}
DD_*(G)\cdot RDD_*(G) &= \left[\sum_{\{u,v\}\subseteq V(G)} [\deg_G(u)\ \deg_G(v)]\mathrm{dist}_G(u,v)\right] \\
&\times \left[\sum_{\{u,v\}\subseteq V(G)} [\deg_G(u)\ \deg_G(v)]\frac{1}{\mathrm{dist}_G(u,v)}\right] \\
&\ge \left[\sum_{\{u,v\}\subseteq V(G)} [\deg_G(u)\ \deg_G(v)]\right]^2 \\
&= \left[\sum_{uv\in E(G)} [\deg_G(u)\ \deg_G(v)] + \sum_{uv\in E(\overline{G})} [\deg_G(u)\ \deg_G(v)]\right]^2 \\
&= [M_2(G) + \overline{M}_2(G)]^2\ .
\end{aligned}$$

Thus $RDD_*(G) \ge \frac{[M_2(G)+\overline{M}_2(G)]^2}{DD_*(G)}$, with equality if and only if $G \cong K_n$. □

Theorem 4. Let G be a connected graph of order n. Then

$$RDD_*(G) \le M_2(G) + \overline{M}_2(G)$$

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

Proof. From $1/\mathrm{dist}_G(u,v) \le 1$ it follows that

$$\begin{aligned}
RDD_*(G) &\le \sum_{\{u,v\}\subseteq V(G)} [\deg_G(u)\deg_G(v)] \\
&= \sum_{uv\in E(G)} [\deg_G(u)\deg_G(v)] + \sum_{uv\in E(\overline{G})} [\deg_G(u)\deg_G(v)] \\
&= M_2(G) + \overline{M}_2(G)\ .
\end{aligned}$$

Thus $RDD_*(G) \leq M_2(G) + \overline{M}_2(G)$, with equality if and only if $\mathrm{dist}_G(u,v) = 1$ for any pair of vertices u and v in G, or equivalently, $G \cong K_n$. □

Theorem 5. Let G be a connected graph of order n. Then

$$\delta(G)^2 H(G) \leq RDD_*(G) \leq \triangle(G)^2 H(G)$$

with equality (on both sides) if and only if G is a regular graph.

Proof. It is obvious that $\delta(G) \leq \deg_G(u) \leq \triangle(G)$ for any vertex u in G. Hence,

$$\delta(G)^2 \sum_{\{u,v\}\subseteq V(G)} \frac{1}{\mathrm{dist}_G(u,v)} \leq RDD_*(G) \leq \triangle(G)^2 \sum_{\{u,v\}\subseteq V(G)} \frac{1}{\mathrm{dist}_G(u,v)}$$

implying the proof, with equality if and only if G is regular. □

3.2. Relation with matching and independence number

A *matching* of a graph G is a set of edges with no shared endpoints. A *maximal matching* in a graph is a matching whose cardinality cannot be increased by adding an edge. The *matching number* $\beta(G)$ is the number of edges in a maximum matching.

A component of a graph is said to be *odd* (resp., *even*) if it has odd (resp., even) number of vertices. Indicate the number of odd components by $o(G)$.

The following is an immediate consequence of the Tutte–Berge formula [24].

Lemma 2. (Lovász [24]) Let G be a connected graph of order n. Then

$$n - 2\beta = \max\{o(G - X) - |X| : X \subset V\} .$$

Lemma 3. (Hacke [15]) The solutions of the real coefficient quartic equation $ax^4 + bx^3 + cx^2 + dx + e = 0$ $(a \neq 0)$ are given by:

$$x_1 = -\frac{b}{4a} + \frac{1}{2}\sqrt{\frac{b^2}{4a^2} - \frac{2c}{3a} + \frac{\sqrt[3]{2}A}{3aB} + \frac{B}{3\sqrt[3]{2}a}} - \frac{1}{2}\sqrt{\frac{b^2}{2a^2} - \frac{4c}{3a} - \frac{\sqrt[3]{2}A}{3aB} - \frac{B}{3\sqrt[3]{2}a} + \frac{C}{4a^3\sqrt{\frac{b^2}{4a^2} - \frac{2c}{3a} + \frac{\sqrt[3]{2}A}{3aB} + \frac{B}{3\sqrt[3]{2}a}}}}$$

$$x_2 = -\frac{b}{4a} + \frac{1}{2}\sqrt{\frac{b^2}{4a^2} - \frac{2c}{3a} + \frac{\sqrt[3]{2}A}{3aB} + \frac{B}{3\sqrt[3]{2}a}} + \frac{1}{2}\sqrt{\frac{b^2}{2a^2} - \frac{4c}{3a} - \frac{\sqrt[3]{2}A}{3aB} - \frac{B}{3\sqrt[3]{2}a} + \frac{C}{4a^3\sqrt{\frac{b^2}{4a^2} - \frac{2c}{3a} + \frac{\sqrt[3]{2}A}{3aB} + \frac{B}{3\sqrt[3]{2}a}}}}$$

$$x_3 = -\frac{b}{4a} - \frac{1}{2}\sqrt{\frac{b^2}{4a^2} - \frac{2c}{3a} + \frac{\sqrt[3]{2}A}{3aB} + \frac{B}{3\sqrt[3]{2}a}} + \frac{1}{2}\sqrt{\frac{b^2}{2a^2} - \frac{4c}{3a} - \frac{\sqrt[3]{2}A}{3aB} - \frac{B}{3\sqrt[3]{2}a} - \frac{C}{4a^3\sqrt{\frac{b^2}{4a^2} - \frac{2c}{3a} + \frac{\sqrt[3]{2}A}{3aB} + \frac{B}{3\sqrt[3]{2}a}}}}$$

$$x_4 = -\frac{b}{4a} - \frac{1}{2}\sqrt{\frac{b^2}{4a^2} - \frac{2c}{3a} + \frac{\sqrt[3]{2}A}{3aB} + \frac{B}{3\sqrt[3]{2}a}} - \frac{1}{2}\sqrt{\frac{b^2}{2a^2} - \frac{4c}{3a} - \frac{\sqrt[3]{2}A}{3aB} - \frac{B}{3\sqrt[3]{2}a} - \frac{C}{4a^3\sqrt{\frac{b^2}{4a^2} - \frac{2c}{3a} + \frac{\sqrt[3]{2}A}{3aB} + \frac{B}{3\sqrt[3]{2}a}}}}$$

where $A = c^2 - 3bd + 12ae$, $B = \sqrt[3]{D + \sqrt{-4A^3 + D^2}}$, $C = -b^3 + 4abc - 8a^2d$, and $D = 2c^3 - 9bcd + 27ad^2 + 27b^2e - 72ace$.

Let $\mathcal{Q}_1(n, \beta)$ denote the class of connected graphs of order n with matching number β.

Theorem 6. Let G be a connected graph of order $n \geq 4$ with matching number $\beta \in [2, \lfloor \frac{n}{2} \rfloor]$. Let σ_1, σ_2, and σ_3 be the positive roots of the equation

$$\frac{31}{4}x^4 + \frac{6n-101}{4}x^3 - \frac{7n^2-33n-74}{4}x^2 + \frac{n^2-20n-2}{2}x + \frac{5n^2+n}{2} = 0\,.$$

Each of the following holds:

(**a**) If $\beta = \lfloor \frac{n}{2} \rfloor$, then $RDD_*(G) \leq n(n-1)^2$, with equality if and only if $G \cong K_n$.

(**b**) If $\beta \in (\sigma_2, \sigma_3) \cup (\sigma_4, \lfloor \frac{n}{2} \rfloor - 1)$, then

$$RDD_*(G) \leq 8\beta^4 - 24\beta^3 + (6n+19)\beta^2 - \frac{18n+3}{2}\beta + \frac{5n^2+n}{4}$$

with equality if and only if $G \cong K_1 + (K_{2\beta-1} \cup \overline{K_{n-2\beta}})$.

(**c**) If $\beta = \sigma_i$ for $i = 1, 2, 3$, then

$$\begin{aligned} RDD_*(G) &\leq 8\beta^4 - 24\beta^3 + (6n+19)\beta^2 - \frac{18n+3}{2}\,'\beta + \frac{5n^2+n}{4} \\ &= \frac{1}{4}\beta^4 - \frac{6n-5}{4}\beta^3 + \frac{7n^2-9n+2}{4}\beta^2 - \frac{n^2-2n+1}{2}\beta \end{aligned}$$

with equality if and only if $G \cong K_\beta + \overline{K_{n-\beta}}$ or $G \cong K_1 + (K_{2\beta-1} \cup \overline{K_{n-2\beta}})$.

(**d**) If $\beta \in [2, \sigma_2] \cup [\sigma_3, \sigma_4]$, then

$$RDD_*(G) \leq \frac{1}{4}\beta^4 - \frac{6n-5}{4}\beta^3 + \frac{7n^2-9n+2}{4}\beta^2 - \frac{n^2-2n+1}{2}\beta$$

with equality if and only if $G \cong K_\beta + \overline{K_{n-\beta}}$.

Proof. Let G' be a connected graph with maximum RDD_*-value in $\mathcal{Q}_1(n, \beta)$. By Lemma 2, there exists a vertex subset $X' \subset V(G')$ such that

$$n - 2\beta = \max\{o(G' - X) - |X| : X \subset V\} = o(G' - X') - |X'|\,.$$

For simplicity, let $|X'| = s$ and $o(G' - X') = t$. Then $n - 2\beta = t - s$.

Case I. $s = 0$.

It follows that $G' - X' = G'$ and then $n - 2\beta = t \leq 1$ since G is connected. If $t = 0$, then G' is an even graph. Then $\beta = n/2$, by Lemma 1, and we obtain that $G' \cong K_n$ and $RDD_*(G) = \frac{n(n-1)^3}{2}$. If $t = 1$, then $\beta = \frac{n-1}{2}$. As before, $RDD_*(G) = \frac{n(n-1)^3}{2}$.

Case II. $s \geq 1$.

Consequently, $t \geq 1$. Otherwise, $t = 0$, then $n - 2\beta = -s < 0$, we have $\beta > \frac{n}{2}$, which contradicts the condition $\beta \in [2, \lfloor n/2 \rfloor]$. Let $G_1^o, G_2^o, \ldots, G_t^o$ be all odd components of $G' - X'$. In order to obtain our result, we state and prove the following three claims.

Claim 1. There is no even component in $G' - X'$.

Assume the contrary, let G^e be an even component. Then the link $(G^e \sim G_i^o)(a \cdot b)$, obtained by joining a vertex $a \in V(G^e)$ and $b \in V(G_i^o)$, is also an odd component in $G' - X'$. We denote such a graph by G'', for which $n - 2\beta(G'') \geq o(G'' - X') - |X'| = o(G' - X') - |X'|$ holds, i.e., $\beta(G'') \leq \beta$, implying that $G'' \in \mathcal{Q}(n, \beta)$, which contradicts to the choice of G'. □

Claim 2. Each odd component G_i^o $(1 \leq i \leq t)$, and the graph induced by X', are complete.

Assume that G_i^o is not complete. Then there must exist two non-adjacent vertices u, v in G_i^o. By Lemma 1, one can get a graph $G' + uv$, which increases the RDD_*-value. This again is a contradiction with the choice of G'. Similarly, we can prove that X' is complete. □

Claim 3. Each vertex of G_i^o is adjacent to those of X'.

This follows by a similar discussion, whose details we skip. □

Now we continue our proof. Without loss of generality, we let $n_i = |V(G_i^o)|$ for $i = 1, 2, \ldots, t$. Then by Claims 1, 2, and 3 we have

$$G' = K_s + (K_{n_1} \cup K_{n_2} \cup \cdots \cup K_{n_t}) .$$

Let $\widehat{RDD}_*(G_1, G_2)$ denote the contribution to the RDD_*-value between vertices of G_1 and those of G_2. Then we have

$$\begin{aligned}
\widehat{RDD}_*(K_{n_i}, K_{n_i}) &= \frac{1}{2}\Big[n_i^4 + (2s-3)n_i^3 + (s^2 - 4s + 3)n_i^2 - (s-1)^2 n_i\Big] \\
\widehat{RDD}_*(K_{n_i}, K_{n_j}) &= \frac{1}{2} n_i\, n_j (n_i + s - 1)(n_j + s - 1) \\
\widehat{RDD}_*(K_{n_i}, K_s) &= s(n-1)n_i^2 + s(s-1)(n-1)n_i \\
\widehat{RDD}_*(K_s, K_s) &= \frac{1}{2} s(s-1)(n-1)^2 .
\end{aligned}$$

Hence, the reciprocal sum–degree distance of G' can be represented as

$$\begin{aligned} RDD_*(G') &= \sum_{i=1}^{t} \widehat{RDD}_*(K_{n_i}, K_{n_i}) + \sum_{i=1}^{t} \widehat{RDD}_*(K_{n_i}, K_s) \\ &+ \sum_{i<j} \widehat{RDD}_*(K_{n_i}, K_{n_j}) + \widehat{RDD}_*(K_s, K_s) \\ &= \frac{1}{2}\sum_{i=1}^{t} n_i^4 + \frac{1}{2}(2s-3)\sum_{i=1}^{t} n_i^3 + \frac{1}{2}(s^2+(2n-6)s+3)\sum_{i=1}^{t} n_i^2 \\ &+ \frac{1}{2}((2n-3)s^2+2ns-1)\sum_{i=1}^{t} n_i + \frac{1}{2}s(s-1)(n-1)^2 \\ &+ \frac{1}{2}\sum_{i<j} n_i n_j (n_i+s-1)(n_j+s-1)\,. \end{aligned}$$

Assume that $1 \le n_1 \le n_2 \le \cdots \le n_t$. Let

$$G'' = K_s + (K_{n_1} \cup K_{n_2} \cup \cdots \cup K_{n_i-1} \cup \cdots \cup K_{n_j+1} \cup \cdots \cup K_{n_t})\,.$$

Then $RDD_*(G') - RDD_*(G'') < 0$. To see this, it is sufficient to prove Claim 4 below, which can be verified by the transformation $(n_i, n_j) \to (n_i - 1, n_j + 1)$.

Claim 4. Each of the following functions

(**a**) $\mathrm{F}_1(n_1, n_2, \ldots, n_t) = n_1^4 + n_2^4 + \cdots + n_t^4$

(**b**) $\mathrm{F}_2(n_1, n_2, \ldots, n_t) = n_1^3 + n_2^3 + \cdots + n_t^3$

(**c**) $\mathrm{F}_3(n_1, n_2, \ldots, n_t) = n_1^2 + n_2^2 + \cdots + n_t^2$

(**d**) $\mathrm{F}_4(n_1, n_2, \ldots, n_t) = \sum_{i<j} n_i n_j (n_i + s - 1)(n_j + s - 1)$

increases by replacing every pair (n_i, n_j) by $n_i - 1, n_j + 1$.

Proof of Claim 4. We will present the proof of parts (**a**) and (**d**), respectively. The other two parts can be verified by similar arguments.

Let $\mathcal{R}_1(n_i, n_j) = \mathrm{F}_1(n_1, n_2, \ldots, n_i, \ldots, n_j, \ldots, n_t)$. Then

$$\mathcal{R}_1(n_i, n_j) - \mathcal{R}_1(n_i - 1, n_j + 1) = 4(n_i^2 + n_j^2)(n_i - n_j - 6) + 4(n_i - n_j)(n_i n_j + 1) - 2 < 0\,.$$

This implies that the transformation $(n_i, n_j) \to (n_i - 1, n_j + 1)$ will increase the value of $\mathcal{R}_1$.

Without loss of generality, we may assume that $\mathcal{R}_2(n_k, n_l) = \mathrm{F}_1(n_1, n_2, \ldots, n_k, \ldots, n_l, \ldots, n_t)$. Then

$$\begin{aligned} \mathcal{R}_2(n_1, n_2) &- \mathcal{R}_2(n_1 - 1, n_2 + 1) \\ &= (n_1 - n_2 - 1)[2n_3(n_3 + s - 1) + 2n_t(n_t + s - 1)] \\ &+ (n_1 - n_2 - 1)[-n_1 n_2 - (n_1 + s - 1)(n_2 + s - 1) - (n_1 - n_2 - 1)] \\ &\doteq (n_1 - n_2 - 1)Q(s)\,. \end{aligned}$$

The first derivative of $Q(s)$ is $Q'(s) = -s^2 + (2n_3 + 2n_t - n_1 - n_2 + 2)s + 2n_3^2 + 2n_t^2 - 2n_3 - 2n_t - 2n_1 n_2 + 2n_2$. It is easy to prove that $Q'(s) > 0$ and $Q(s) > 0$ for $1 \le s \le \frac{2n_3+2n_t-n_1-n_2+2}{2}$. By the same arguments, we can obtain the proof of (**d**). □

By repeatedly using Claim 4, we find that $RDD_*(G')$ attains maximum if and only if $n_1 = n_2 = \cdots = n_{t-1} = 1$ and $n_t = 2\beta - 2s + 1$. It follows that $G' \cong K_s + (K_{2\beta-2s+1} \cup \overline{K_{n+s-2\beta-1}})$.

Simple calculations show that

$$\begin{aligned}
\widehat{RDD}_*(K_{2\beta-2s+1}, K_{2\beta-2s+1}) &= \binom{2\beta-2s+1}{2}(2\beta-s)^2 \\
\widehat{RDD}_*(\overline{K_{n+s-2\beta-1}}, \overline{K_{n+s-2\beta-1}}) &= \frac{1}{2}\binom{n+s-2\beta-1}{2}s^2 \\
\widehat{RDD}_*(K_{2\beta-2s+1}, \overline{K_{n+s-2\beta-1}}) &= \frac{1}{2}(2\beta-2s+1)(n+s-2\beta-1)(2\beta-s)s \\
\widehat{RDD}_*(K_s, K_{2\beta-2s+1}) &= s(2\beta-2s+1)(2\beta-s)(n-1) \\
\widehat{RDD}_*(K_s, \overline{K_{n+s-2\beta-1}}) &= s(n+s-2\beta-1)(n-1)s \\
\widehat{RDD}_*(K_s, K_s) &= \frac{1}{2}s(s-1)(n-1)^2 .
\end{aligned}$$

Taking the above into account, it follows that

$$\begin{aligned}
RDD_*(G') &= \widehat{RDD}_*(K_{2\beta-2s+1}, K_{2\beta-2s+1}) + \widehat{RDD}_*(\overline{K_{n+s-2\beta-1}}, \overline{K_{n+s-2\beta-1}}) \\
&+ \widehat{RDD}_*(K_{2\beta-2s+1}, \overline{K_{n+s-2\beta-1}}) + \widehat{RDD}_*(K_s, K_{2\beta-2s+1}) \\
&+ \widehat{RDD}_*(K_s, \overline{K_{n+s-2\beta-1}}) + \widehat{RDD}_*(K_s, K_s) \\
&= \frac{13}{4}s^4 + \frac{18n-72\beta-25}{4}s^3 + \left[35\beta^2 + \frac{39-24n}{2}\beta + \frac{7n^2-21n+14}{4}\right]s^2 \\
&- \left[28\beta^3 - (6n-16)\beta^2 - (3n-3)\beta + \frac{n^2-2n+1}{2}\right]s + 8\beta^4 + 4\beta^3 .
\end{aligned}$$

Analyzing the function Φ on s

$$\begin{aligned}
\Phi(s) &= \frac{13}{4}s^4 + \frac{18n-72\beta-25}{4}s^3 + \left[35\beta^2 + \frac{39-24n}{2}\beta + \frac{7n^2-21n+14}{4}\right]s^2 \\
&- \left[28\beta^3 - (6n-16)\beta^2 - (3n-3)\beta + \frac{n^2-2n+1}{2}\right]s + 8\beta^4 + 4\beta^3
\end{aligned}$$

it follows that $s \leq \beta$, since $t - s = n - 2\beta \geq t + s - 2\beta$. By taking derivatives, we have

$$\begin{aligned}
\Phi'(s) &= 13s^3 + \frac{54n-216\beta-75}{4}s^2 + \left[70\beta^2 + \frac{39-24n}{2}\beta + \frac{7n^2-21n+14}{2}\right]s \\
&- \left[28\beta^3 - (6n-16)\beta^2 - (3n-3)\beta + \frac{n^2-2n+1}{2}\right] \\
\Phi''(s) &= 39s^2 + \frac{54n-216\beta-75}{2}s + \left[70\beta^2 + (39-24n)2\beta + \frac{7n^2-21n+14}{2}\right].
\end{aligned}$$

In what follows, we establish:

Claim 5. $\Phi''(s) > 0$.

Proof of Claim 5. The discriminant of $\Phi''(s)$ is

$$\triangle_{\Phi''} = 744\beta^2 - (2088n - 2016)\beta + 183n^2 - 387n + \frac{1257}{4} = Q_1(\beta) .$$

Consider now the function

$$Q_1(\beta) = 744\beta^2 - (2088n - 2016)\beta + 183n^2 - 387n + \frac{1257}{4} .$$

It is easy to verify that

$$\triangle_{Q_1} = 3815136n^2 - 7267104n + 3129048 = Q_2(n) .$$

The discriminant of $Q_2(n)$ is $\triangle_{Q_2} = 5.28108 \times 10^{13} - 4.775097 \times 10^{13} > 0$. Thus, the greatest positive root of $Q_2(n) = 0$ is $n_0 = \frac{7267104+\sqrt{\triangle_{Q_2}}}{7630272}$. It is obvious that $\triangle_{Q_1} = Q_2(n) > 0$ when $n > n_0$. In an analogous manner, we get the greatest root of $Q_1(\beta) = 0$ as

$$\beta_+ = \frac{2088n - 2016 + \sqrt{Q_2(n)}}{744 \times 2} > \frac{2088n + \sqrt{2214144n}}{744 \times 2} > n > \left\lfloor \frac{n}{2} \right\rfloor - 1 .$$

For $\beta \in [2, \lfloor \frac{n}{2} \rfloor - 1]$, we have $Q_1(\beta) = \triangle_{\Phi''} < 0$, which completes the proof of Claim 5. □

By Claim 5, we know that $\Phi(s)$ is a strictly convex function for $s \leq \beta$, and that its maximum is attained at $s = 1$ or $s = \beta$:

$$\Phi(1) = 8\beta^4 - 24\beta^3 + (6n + 19)\beta^2 - \frac{18n + 3}{2}\beta + \frac{5n^2 + n}{4}$$

and

$$\Phi(\beta) = \frac{1}{4}\beta^4 - \frac{6n - 5}{4}\beta^3 + \frac{7n^2 - 9n + 2}{4}\beta^2 - \frac{n^2 - 2n + 1}{2}\beta .$$

After subtraction, we obtain

$$\Phi(1) - \Phi(\beta) = \frac{31}{4}\beta^4 + \frac{6n - 101}{4}\beta^3 - \frac{7n^2 - 33n - 74}{4}\beta^2 + \frac{n^2 - 20n - 2}{4}\beta + \frac{5n^2 + n}{2} .$$

Now, let us consider the function Ψ on β

$$\Psi(\beta) = \frac{31}{4}\beta^4 + \frac{6n - 101}{4}\beta^3 - \frac{7n^2 - 33n - 74}{4}\beta^2 + \frac{n^2 - 20n - 2}{4}\beta + \frac{5n^2 + n}{2} .$$

It is easy to see that $\Psi(2) = -\frac{1}{2}(7n^2 - 51n + 12) < 0$ since $7n^2 - 51n + 12 > 0$ for $n > \frac{51+\sqrt{2265}}{14}$. Note that $\Psi(\beta)$ is continuous on the interval $[2, \lfloor \frac{n}{2} \rfloor - 1]$. Then by Lemma 3, we have $\Psi(\beta) < 0$ for $[2, \sigma_2] \cup [\sigma_3, \sigma_4]$; $\Psi(\beta) > 0$ for $(\sigma_2, \sigma_3) \cup (\sigma_4, \lfloor \frac{n}{2} \rfloor - 1)$. This completes the proof of Theorem 6. □

Example 1. If $n = 21$ and $\beta = 2$, then $K_2 + \overline{K_{19}} \in Q_1(21, 2)$, and $RDD_*(K_2 + \overline{K_{19}}) = 2262$. The formula of part (**d**) in Theorem 6 also gives upper bound of 2262.

A subset I of $V(G)$ is said to be an *independent set* of the graph G if the subgraph induced by I is an empty graph. Then $\alpha = \max\{|I| : I \text{ is an independent set of } G\}$ is said to be the *independence number* of G.

Let $Q_2(n, \alpha)$ be the class of connected graphs of order n with independence number α.

Theorem 7. Let $G \in Q_2(n, \alpha)$. Then

$$RDD_*(G) \leq \frac{1}{4}\alpha^4 + \frac{2n - 5}{4}\alpha^3 - \frac{5n^2 - 6n - 2}{4}\alpha^2 + \frac{5n^2 - 8n + 2}{4}\alpha + \frac{n(n-1)^3}{2}$$

with equality if and only if $G \cong \overline{K_\alpha} + K_{n-\alpha}$.

Proof. Let G' be a connected graph with maximum RDD_*-value in $\mathcal{Q}_2(n,\alpha)$. Let I be a maximal independent set in G' with $|I| = \alpha$. Note that by Lemma 1, adding edges into a graph will increase its RDD_*-value. Therefore, each vertex u in I must be adjacent to those in $G' - I$. In addition, the subgraph induced by vertices in $G' - I$ is complete in G'. Hence, $G \cong \overline{K_\alpha} + K_{n-\alpha}$. By elementary computation we obtain that $RDD_*(\overline{K_\alpha} + K_{n-\alpha})$ coincides with the right–hand side of Eq. (8), which completes the proof. □

3.3. Relation with vertex–connectivity

Lemma 4. Let n, x, y, and κ be four positive integers such that $y > x$, $x + y = n - \kappa$ and $\kappa < \frac{4n-2+\sqrt{31n^2-64n+4}}{3}$. Then the function

$$\begin{aligned} f(x,y) &= 2(x^3-y^3)+3(x^2+y^2)+2(x-y)+\frac{2\kappa-3}{2}[3(x^2-y^2)+3(x+y)] \\ &+ xy^2-x^2y+\frac{1}{2}(x-y)^2-xy+x-y \\ &+ \frac{2\kappa^2+(3n-11)\kappa+n-7}{2}(x-y+1)+\frac{3}{2} \end{aligned}$$

has positive value at $x = \frac{n-\kappa-1}{2}$.

Proof. Let $p = n - \kappa$ for simplicity. Then

$$\begin{aligned} Q_1(x) = f(x,p-x) &= 6x^3+(9-9p)x^2+[7p^2-18p+6p\kappa+n-1+2\kappa^2+(3n-11)\kappa]x \\ &- 2p^3+(8-3\kappa)p^2-[\kappa^2+\frac{1}{2}(3n-17)\kappa+\frac{1}{2}n+4]p \\ &+ \frac{1}{2}[2\kappa^2+(3n-11)\kappa+n-4]\,. \end{aligned}$$

The first and second derivatives of $Q_1(x)$ are $Q_1'(x) = 18x^2+(18-18p)x+7p^2-18p+6p\kappa+n-1+2\kappa^2+(3n-11)\kappa$ and $Q_1''(x) = 36x + 18 - 18p$. We distinguish the following two cases.

Case 1. $x \geq \frac{p-1}{2}$.

In this case, $Q_1''(x) = 36x+18-18p > 0$, which shows that $Q_1'(x)$ is an increasing function for $x \geq \frac{p-1}{2}$. Then $Q_1'(x) \geq Q_1'(\frac{p-1}{2}) = -\frac{3}{2}\kappa^2 + (4n-2)\kappa + \frac{5}{2}n^2 - 8n$. It is easy to verify that $Q_1'(\frac{p-1}{2}) > 0$ for $\kappa < \frac{4n-2+\sqrt{31n^2-64n+4}}{3}$. This implies that $Q_1(x)$ is increasing and therefore $Q_1(x) \geq Q_1(\frac{p-1}{2})$. By elementary calculations, we get $Q_1(\frac{p-1}{2}) = \kappa^2 + \frac{1}{2}(3n-11)\kappa + 2 > 0$.

Case 2. $2 \leq x < \frac{p-1}{2}$.

In this case, $Q_1''(x) = 36x + 18 - 18p < 0$, which shows that $Q_1'(x)$ is a decreasing function for $2 \leq x < \frac{p-1}{2}$. Then $Q_1'(x) \geq Q_1'(\frac{p-1}{2}) = -\frac{3}{2}\kappa^2+(4n-2)\kappa+\frac{5}{2}n^2-8n$. It is easy to verify that $Q_1'(\frac{p-1}{2}) > 0$ for $\kappa < \frac{4n-2+\sqrt{31n^2-64n+4}}{3}$. This implies that $Q_1(x)$ is increasing and therefore $Q_1(x) \geq Q_1(\frac{p-1}{2})$. By elementary calculations, we get $Q_1(\frac{p-1}{2}) = \kappa^2 + \frac{1}{2}(3n-11)\kappa + 2 > 0$.

Based on the discussions above, $Q_1(x)$ attains a positive value at $x = \frac{n-\kappa-1}{2}$. □

The *vertex–connectivity* $\kappa(G)$ of a connected graph G is the minimum size of a vertex set S such that $G - S$ is disconnected or has one vertex.

Let $\mathcal{Q}_3(n,\kappa)$ be the class of connected graphs of order n with vertex-connectivity κ.

Theorem 8. Let $G \in \mathcal{Q}_3(n,\kappa)$. Then

$$RDD_*(G) \leq \frac{1}{2}n^4 - \frac{7}{2}n^3 + \frac{\kappa^3-\kappa^2+3\kappa+18}{2}n^2 + \frac{\kappa^3-11\kappa-20}{2}n + \frac{\kappa^2+9\kappa+8}{2}$$

with equality if and only if $G \cong K_\kappa + (K_1 \cup K_{n-\kappa-1})$.

Proof. Let G' be a connected graph with maximum RDD_*-value in $\mathcal{Q}_3(n,\kappa)$. Let C be a vertex-cut in G' with $|C| = \kappa$ and $G_1, G_2, \ldots, G_t$ $(t \geq 2)$ be the components of $G' - C$. By Lemma 1, we have $t = 2$ and each G_i for $i = 1, 2$ is complete. Otherwise, we could get a new graph with greater RDD_*-value by adding edges, which would contradict to the choice of G'. The same argument leads us to the conclusion that each G_i is complete for $i = 1, 2$, that the subgraph of G' induced by C is complete, and that each vertex of $G_1 \cup G_2$ is adjacent to that of C.

Let $n_1 = |V(G_1)|$, $n_2 = |V(G_2)|$, then $n = n_1 + n_2 + \kappa$. From the above argument, we know that $G' \cong K_\kappa + (K_{n_1} \cup K_{n_2})$ and that for $x \in V(G_1)$, $y \in V(G_2)$, $z \in C$, we have $\deg(x) = \kappa + (n_1 - 1)$, $\deg(y) = \kappa + (n_2 - 1)$, and $\deg(z) = n - 1$.

Without loss of generality, we assume that $n_2 \geq n_1 \geq 2$. If $n_1 = 1$, then the result follows directly. By elementary computation, we get

$$\begin{aligned} RDD_*(G') &= \frac{1}{2}(n_1^4 + n_2^4) + \left(k - \frac{3}{2}\right)(n_1^3 + n_2^3) + \frac{1}{2}n_1^2 n_2^2 \\ &- \frac{1}{2}[2\kappa^2 + (3n-11)\kappa + n - 7]n_1 n_2 + \frac{1}{2}\kappa(\kappa-1)(n-1)^2 \\ &+ \frac{1}{2}(\kappa^2 - 4\kappa + 3)(n-\kappa)^2 - \frac{1}{2}(n-\kappa)(\kappa-1)^2 \\ &+ \kappa(\kappa-1)(n-1)(n-\kappa) + \kappa(n-1)(n-\kappa)^2 . \end{aligned}$$

Let $G'' \cong K_\kappa + (K_{n_1-1} \cup K_{n_2+1})$. We will confirm that replacing every pair (n_i, n_j) by $(n_i - 1, n_j + 1)$, the RDD_*-value will be increased. Actually,

$$\begin{aligned} RDD_*(G'') - RDD_*(G') &= \frac{1}{2}[4(n_2^3 - n_1^3) + 6(n_1^2 + n_2^2) + 4(n_2 - n_1) + 2] \\ &+ \left(\kappa - \frac{3}{2}\right)[3(n_2^2 - n_1^2) + 3(n_1 + n_2)] \\ &+ \frac{1}{2}[2n_1^2 n_2 - 2n_1 n_2^2 + (n_1 - n_2)^2 - 2n_1 n_2 + 2(n_2 - n_1) + 1] \\ &- \frac{1}{2}[2\kappa^2 + (3n-11)\kappa + n - 7](n_1 - n_2 - 1) . \end{aligned}$$

Let $n_2 = x, n_1 = y$. Then by Lemma 4, $RDD_*(G'') - RDD_*(G') > 0$. This implies that $G' \cong K_\kappa + (K_1 \cup K_{n-\kappa-1})$. By direct computation we get

$$\begin{aligned} RDD_*(K_\kappa + (K_1 \cup K_{n-\kappa-1})) &\leq \frac{1}{2}n^4 - \frac{7}{2}n^3 + \frac{\kappa^3 - \kappa^2 + 3\kappa + 18}{2}n^2 \\ &+ \frac{\kappa^3 - 11\kappa - 20}{2}n + \frac{\kappa^2 + 9\kappa + 8}{2} . \end{aligned}$$

This completes the proof of Theorem 8. □

Example 2. If $(n, \kappa, n_1, n_2) = (3, 1, 1, 1)$, then $G' = P_3 \in \mathcal{Q}_3(3, 1)$ and $RDD_*(G') = \frac{9}{2}$. The formula of right side in Theorem 8 also gives upper bound of $\frac{9}{2}$.

4. A Nordhaus–Gaddum–Type Relation for RDD_*

A *coloring* of a graph G is an assignment of colors to its vertices such that two adjacent vertices have different colors. The minimum number of colors in a coloring of G is said to be its *chromatic number* and is denoted by $\chi(G)$.

In 1956, Nordhaus and Gaddum [27] studied the chromatic number in a graph G and in its complement $\overline{G}$ together. They proved:

Theorem 9. (Nordhaus and Gaddum, [27]) Let G be a connected graph of order n. Then

$$2\sqrt{n} \leq \chi(G) + \chi(\overline{G}) \leq n+1 \qquad \text{and} \qquad n \leq \chi(G)\cdot\chi(\overline{G}) \leq \frac{(n+1)^2}{4}\,.$$

Furthermore, these bounds are best possible for infinitely many values of n.

Since then, any bound on the sum and/or the product of an invariant in a graph G and the same invariant in the complement $\overline{G}$ is called a *Nordhaus–Gaddum–type inequality* or Nordhaus–Gaddum–type relation.

Many Nordhaus–Gaddum–type results have been obtained so far; see the recent survey [3]. Below we state one more, pertaining to the reciprocal product–degree distance.

Zhang and Wu [36] obtained a Nordhaus–Gaddum–type result for the Wiener index. Three years later, Zhou et al. gave the following analogous result for the Harary index [37].

Lemma 5. (Zhou et al. [37]) Let G be a connected graph of order $n \geq 5$ with connected complement. Then

$$1 + \frac{(n-1)^2}{2} + n\sum_{i=1}^{n-1}\frac{1}{i} \leq H(G) + H(\overline{G}) \leq \frac{3n(n-1)}{4}$$

with left equality if and only if $G \cong P_n$ or $G \cong \overline{P_n}$, and with right equality if and only if both G and $\overline{G}$ have diameter 2.

Let $\mathcal{P}_{n,\kappa}$ be the set of connected graphs of order n whose complement is also connected, such that $\operatorname{diam}(G) = \operatorname{diam}(\overline{G}) = \kappa$ for $\kappa \geq 2$.

The main result in this section can be stated as:

Theorem 10. Let G be a connected graph of order $n \geq 5$ with connected complement. Let $\mathcal{R}_-(\delta) = \min\{\delta(G)^2, \delta(\overline{G})^2\}$ and $\mathcal{R}_+(\delta) = \max\{\triangle(G)^2, \triangle(\overline{G})^2\}$. Then

$$\mathcal{R}_-(\delta)\left[1 + \frac{(n-1)^2}{2} + n\sum_{i=1}^{n-1}\frac{1}{i}\right] \leq RDD_*(G) + RDD_*(\overline{G}) \leq \frac{3n(n-1)}{4}\mathcal{R}_+(\delta)$$

with left equality if and only if $G \cong \overline{P_n}$, and with right equality if and only if $\mathcal{P}_{n,2}$.

Proof. Since G and $\overline{G}$ are connected, by Theorem 5 and Lemma 5,

$$\begin{aligned} RDD_*(G) + RDD_*(\overline{G}) &\leq \triangle(G)^2\, H(G) + \triangle(\overline{G})^2\, H(\overline{G}) \\ &\leq \max\{\triangle(G)^2, \triangle(\overline{G})^2\}(H(G) + H(\overline{G})) \\ &\leq \frac{3n(n-1)}{4}\max\{\triangle(G)^2, \triangle(\overline{G})^2\}\,. \end{aligned}$$

with right equality if and only if G and $\overline{G}$ are regular graphs such that $\operatorname{diam}(G) = \operatorname{diam}(G) = 2$, or equivalently, $G \in \mathcal{P}_{n,2}$.

By Theorem 5 and Lemma 5, we also get

$$\begin{aligned} RDD_*(G) + RDD_*(\overline{G}) &\geq \delta(G)^2 H(G) + \delta(\overline{G})^2 H(\overline{G}) \\ &\geq \min\{\delta(G)^2, \delta(\overline{G})^2\}(H(G) + H(\overline{G})) \\ &\geq \min\{\delta(G)^2, \delta(\overline{G})^2\}\left[1 + \frac{(n-1)^2}{2} + n\sum_{i=1}^{n-1}\frac{1}{i}\right]. \end{aligned}$$

with left equality if and only if $G \cong \overline{P_n}$.

This completes the proof of Theorem 10. □

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