On the reciprocal degree distance of graphs with cut vertices or cut edges *

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Abstract: As an additive weight version of the Harary index, the reciprocal degree distance of a simple connected graph G is defined as $RDD(G) = \sum\limits_{\{u,v\}\subseteq V(G)} \frac{d_G(u)+d_G(v)}{d_G(u,v)}$, where $d_G(u)$ is the degree of u and $d_G(u,v)$ is the distance between u and v in G. In this paper, we respectively characterize the extremal graphs with the maximum RDD-value among all the graphs of order n with given number of cut vertices and cut edges. In addition, an upper bound on the reciprocal degree distance in terms of the number of cut edges is provided.

1 Introduction

Chemical graphs are models of molecules in which atoms and chemical bonds are represented by vertices and edges of a graph, respectively. Chemical graph theory is a branch of mathematical chemistry concerning the study of chemical graphs. A graph invariant (also known as molecular descriptor or topological index) is a function on a graph that does not depend on a labelling of its vertices. The chemical information derived through topological index has been found useful in chemical documentation, isomer discrimination, structure property correlations, etc [2]. Hundreds of graph invariants of molecular graphs are studied in chemical graph theory. In this paper, we are interested in a distance-degree-based graph invariant which is called the reciprocal degree distance of a graph.

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Let G be a simple connected graph with vertex set $V(G)$ and edge set $E(G)$. $d_G(v)$ denotes the degree of a vertex v in G and $d_G(u, v)$ denotes the distance between two vertices u and v in G.

For a connected graph G, one of the oldest and well-known distance-based graph invariants is Wiener index, denoted by $W(G)$, which was introduced by Wiener [21] in 1947 and defined as the sum of distances over all unordered vertex pairs in G, i.e.,

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

Another distance-based graph invariant is Harary index, denoted by $H(G)$, which is defined as the sum of reciprocals of distances between all pairs of vertices in G, i.e.

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

In 1994, a degree-weighted version of Wiener index called degree distance or Schultz molecular toplogical index was proposed by Dobrynin and Kochetova [6] and Gutman [8] independently, which is defined for a connected graph G as

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

The interested readers may consult [7, 9, 10] for Wiener index, [5, 11, 16, 20] for Harary index and [3, 4, 13, 17, 18, 19] for degree distance.

Similarly, a degree-weighted version of Harary index called reciprocal degree distance was proposed by Alizadeh et al. [1] in 2013 and Hua and Zhang [12] in 2012 independently, which is defined for a connected graph G as

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

It was shown in [1] that this index can be used as an efficient measuring tool in the study of complex networks.

In general, for a given graph G, $RDD(G)$ is not always easily calculated. So it makes sense to determine the bounds of $RDD(G)$ or to characterize the graphs with extremal reciprocal degree distance among a given class of graphs. In [12], Hua and Zhang established various lower and upper bounds for the reciprocal degree distance among various given classes of graphs including tree, unicyclic graph, cactus and given pendent vertices, independence number, chromatic number, vertex connectivity and edge connectivity. Li and Meng [14] characterized the extremal graphs among n vertex trees with given some graphic parameters such as pendents, matching number, domination number, diameter, vertex bipartition, and determined some sharp upper bounds of trees. Li et al. [15] determined the maximum RDD-value among all the graphs of diameter d and the connected bipartite graphs with given matching number (resp. vertex connectivity). Motivated by the above results, we proceed with the study on the reciprocal degree distance. In this paper, we characterize the unique graph with the maximum RDD-value among all graphs with a given number of cut vertices or edges, and provide an upper bound of the reciprocal degree distance in terms of the number of cut edges.

2 Preliminaries

Let G be a graph, $N_G(v)$ denotes the neighborhood of v in G, so $|N_G(v)| = d_G(v)$. A vertex v of G is called pendent if $d_G(v) = 1$, and the edge incident with v is called a pendent edge of G. A pendent path at v of 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. A cut vertex (edge, respectively) of a graph is a vertex (an edge, respectively) whose removal increases the number of components of the graph. A block of a connected graph is defined to be a maximum connected subgraph without cut vertices. A block containing only one cut vertex is called a pendent block, and a block containing only a unique vertex is called trivial. Denote by $P_s = v_1v_2...v_s$ a path on vertices $v_1, v_2, ..., v_s$ with edges v_iv_{i+1} for $i = 1, 2, ..., s-1$, and denote by K_n a complete graph with order n. For simplicity, we denote by $\mathcal{G}_{n,k}(\overline{\mathcal{G}}_{n,k}$, respectively) the set of graphs of order n with k cut vertices(edges, respectively), and denote by $G_{n,k}$ the graph of order n obtained from the complete graph K_{n-k} by adding $n-k$ paths of almost equal lengths which attached to the different vertices of K_{n-k}, denote by $\overline{G}_{n,k}$ the graph obtained from the complete graph K_{n-k} by attaching k pendent vertices to one vertex of K_{n-k}.

For a subset $V_1 \subset V(G)$, let $G - V_1$ be the subgraph of G obtained by deleting the vertices of V_1 together with the edges incident with them. If $V_1 = \{v\}$, we denote by $G - v$ for simplicity. Similarly, for a subset $E_1 \subset E(G)$, let $G - E_1$ be the subgraph of G obtained by deleting the edges of E_1. For a subset $E_2 \subset E(G^c)$, let $G + E_2$ be the graph obtained from G by adding the edges of E_2, where G^c is the complement of G. If $E_1 = \{e\}$ ($E_2 = \{e\}$, respectively), we denote by $G - e$ ($G + e$, respectively) for simplicity.

Note that in any disconnected graph G, the distance of any two vertices from two distinct components is infinite. Therefore its reciprocal can be viewed as 0. Thus, we can define validly the reciprocals degree distance of disconnected graph G as follows:

$$RDD(G) = \sum_{i=1}^{k} RDD(G_i),$$

where $G_1, G_2, \ldots, G_k$ are the components of G.

Let $D_G(u) = \sum_{v \in V(G) \setminus \{u\}} \frac{1}{d_G(u,v)}$. From [12], we get $RDD(G) = \sum_{u \in V(G)} d_G(u) D_G(u)$.

By a simple analysis, we immediately have the following lemma, which was presented in [12] for a connected graph.

LEMMA 2.1. *Let G be a graph with $u, v \in V(G)$. If $uv \in E(G)$, then $RDD(G) > RDD(G - uv)$. If $uv \notin E(G)$, then $RDD(G) < RDD(G + uv)$.*

3 Maximum reciprocal degree distance of graphs with given number of cut vertices

In this section, we first introduce two edge-grafting transformations to study the mathematical properties of the reciprocal degree distance of G. Then using these mathematical properties, we characterize the extremal graphs with the maximum RDD-value among all the graphs of order n with given number of cut vertices.

LEMMA 3.1. *Let G_1, G_2, P_s be pairwise vertex-disjoint connected graphs, where G_1 contains an edge uv such that $N_{G_1}(u) \setminus \{v\} = N_{G_1}(v) \setminus \{u\} = \{w_1, w_2, \ldots, w_k\}$ ($k \geq 1$), G_2 contains a shortest path $x_1 \ldots x_t$ from x_1 to x_t, $P_s = z_1 z_2 \ldots z_s$, and $t \geq s + 2$. Let G be obtained from G_1, G_2 and P_s by identifying u with x_1 and v with z_1, and let $H = G - \{z_1 w_1, z_1 w_2, \ldots, z_1 w_k\} + \{x_2 w_1, x_2 w_2, \ldots, x_2 w_k\}$, where G and H are shown in Fig. 3.1. Then*

$$RDD(G) < RDD(H).$$

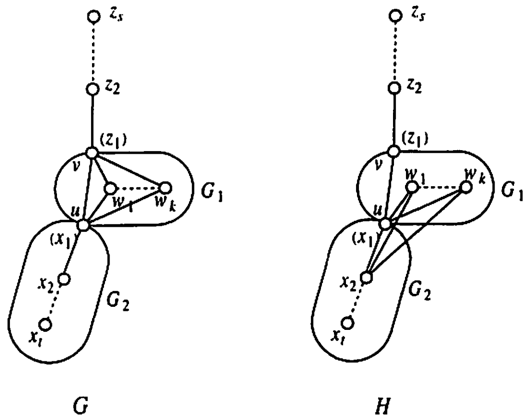

Fig. 3.1 The graphs G and H in Lemma 3.1.

Proof: Let P be the path of G obtained by connecting the paths $x_1 \ldots x_t, uv$ and $z_1 \ldots z_s$, where $u = x_1$ and $v = z_1$. Partition the vertex set of G as $V(G) = (V(G_1)\backslash\{u, v\}) \cup (V(G_2)\backslash\{x_1, \ldots, x_t\} \cup V(P) =: S_1 \cup S_2 \cup S_3$. Then from G to H, the vertices whose degrees changed only are z_1 and x_2: $d_G(z_1) = k + 2$, while $d_H(z_1) = 2$; and $d_G(x_2) + k = d_H(x_2)$. The vertex pairs whose distances changed only are: the distance from any vertex of S_1 to any of S_2 is not increased; the distance from any vertex of S_1 to $z_i (i = 1, 2, \ldots, s)$ of S_3 is increased by 1, and to $x_i (i = 2, 3, \ldots, t)$ is decreased by 1.

(1) Firstly, we consider the vertices of S_1. For any $x \in S_1$, from G to H, the degree of x is unchanged, the distance between x and any other vertex of S_1 is unchanged, the distance between x and any vertex of S_2 is not increased, the distance from x to any of $z_i (i = 1, 2, \ldots, s)$ is increased by 1, and to any of $x_i (i = 2, 3, \ldots, t)$ is decreased by 1, and to the vertex u is unchanged. By the analysis above and letting $d_G(x, u) = m$, we have

$$\begin{aligned} D_H(x) - D_G(x) &\geq \left(\sum_{i=0}^{t-2} \frac{1}{m+i} - \sum_{i=1}^{t-1} \frac{1}{m+i}\right) + \left(\sum_{i=1}^{s} \frac{1}{m+i} - \sum_{i=0}^{s-1} \frac{1}{m+i}\right) \\ &= \frac{1}{m} - \frac{1}{m+t-1} - \frac{1}{m} + \frac{1}{m+s} \\ &> 0. \end{aligned}$$

So, $\sum_{x \in S_1} d_H(x) D_H(x) > \sum_{x \in S_1} d_G(x) D_G(x)$.

(2) Then we consider the vertices of S_2. For any $x \in S_2$, from G to H, the degree of x is unchanged, the distance between x and any other vertex of S_2 is unchanged, the distance between x and any vertex of S_3 is unchanged, while the

distance between x and any vertex of S_1 is not increased. By the analysis above, we have $D_H(x) - D_G(x) \geq 0$. So, $\sum_{x \in S_2} d_H(x)D_H(x) \geq \sum_{x \in S_2} d_G(x)D_G(x)$.

(3) Finally, we consider the vertices of S_3.

From G to H, the degree of vertex u is unchanged, and the distance from u to any other vertex in G is unchanged. So $d_H(u)D_H(u) = d_G(u)D_G(u)$.

From G to H, the degrees of vertices $z_2, z_3, \ldots, z_s$ are unchanged, and for any $z_i (i = 2, \ldots, s)$, the distance between z_i and any vertex of $S_2 \cup S_3$ is unchanged, while the distance between z_i and any vertex of S_1 is increased by 1. Then $D_H(z_i) - D_G(z_i) = \sum_{x \in S_1} \frac{1}{d_G(z_i, x)+1} - \sum_{x \in S_1} \frac{1}{d_G(z_i, x)}$. Hence, $d_G(z_i)D_G(z_i) > d_H(z_i)D_H(z_i)$.

From G to H, the degrees of vertices $x_3, x_4, \ldots, x_t$ are unchanged, and for any $x_i (i = 3, \ldots, t)$, the distance between x_i and any vertex of $S_2 \cup S_3$ is unchanged, while the distance between x_i and any vertex of S_1 is decreased by 1. Then $D_H(x_i) - D_G(x_i) = \sum_{x \in S_1} \frac{1}{d_G(x_i, x)-1} - \sum_{x \in S_1} \frac{1}{d_G(x_i, x)}$. Hence, $d_G(x_i)D_G(x_i) < d_H(x_i)D_H(x_i)$.

Next we compare the change of z_2 and x_3. For any vertex $y \in S_1$, assuming $d_G(u, y) = a$, we have $d_H(y, z_2) = a + 2, d_G(y, z_2) = a + 1, d_H(y, x_3) = a + 1, d_G(y, x_3) = a + 2$. Then

$$\frac{1}{d_H(y, z_2)} - \frac{1}{d_G(y, z_2)} = \frac{1}{a+2} - \frac{1}{a+1} = \frac{-1}{(a+1)(a+2)},$$

$$\frac{1}{d_H(y, x_3)} - \frac{1}{d_G(y, x_3)} = \frac{1}{a+1} - \frac{1}{a+2} = \frac{1}{(a+1)(a+2)}.$$

Notice that $d_G(z_2) = d_H(z_2) = 2, d_G(x_3) = d_H(x_3) \geq 2$, we get

$$d_H(z_2)D_H(z_2) + d_H(x_3)D_H(x_3) \geq d_G(z_2)D_G(z_2) + d_G(x_3)D_G(x_3).$$

Similarly, $d_H(z_i)D_H(z_i) + d_H(x_{i+1})D_H(x_{i+1}) \geq d_G(z_i)D_G(z_i) + d_G(x_{i+1})D_G(x_{i+1})$ for $i = 3, \ldots, s$.

Notice that $t \geq s + 2$, so

$$\sum_{i=2}^{s} d_H(z_i)D_H(z_i) + \sum_{i=3}^{t} d_H(x_i)D_H(x_i) > \sum_{i=2}^{s} d_G(z_i)D_G(z_i) + \sum_{i=3}^{t} d_G(x_i)D_G(x_i).$$

Finally, we prove $d_H(z_1)D_H(z_1) + d_H(x_2)D_H(x_2) > d_G(z_1)D_G(z_1) + d_G(x_2)D_G(x_2)$. Assuming $d_{G_2}(x_2) = l + 2$ $(l \geq 0)$, then we have

$$\begin{aligned}
& (d_H(z_1)D_H(z_1) + d_H(x_2)D_H(x_2)) - (d_G(z_1)D_G(z_1) + d_G(x_2)D_G(x_2)) \\
= \; & 2(D_H(z_1) - D_G(z_1)) + (2 + l)(D_H(x_2) - D_G(x_2)) + k(D_H(x_2) - D_G(z_1)) \\
= \; & \sum_{x \in S_1} [(\tfrac{2}{d_G(x, z_1)+1} - \tfrac{2}{d_G(x, z_1)}) + (\tfrac{2+l}{d_G(x, x_2)-1} - \tfrac{2+l}{d_G(x, x_2)})] + k(D_H(x_2) - D_G(z_1))
\end{aligned}$$

For any $x \in S_1$, assuming $d_G(x,u) = a$, then

$$\frac{1}{d_G(x,z_1)+1} - \frac{1}{d_G(x,z_1)} = \frac{1}{a+1} - \frac{1}{a} = \frac{-1}{a(a+1)},$$

$$\frac{1}{d_G(x,x_2)-1} - \frac{1}{d_G(x,x_2)} = \frac{1}{a} - \frac{1}{a+1} = \frac{1}{a(a+1)}.$$

Since $l \geq 0$, we have

$$\sum_{x \in S_1} [(\frac{2}{d_G(x,z_1)+1} - \frac{2}{d_G(x,z_1)}) + (\frac{2+l}{d_G(x,x_2)-1} - \frac{2+l}{d_G(x,x_2)})] \geq 0.$$

For any $x \in S_1, d_H(x,x_2) = d_G(x,z_1)$. For any $x \in S_2, d_H(x,x_2) \leq d_G(x,z_1)$, so $\frac{1}{d_H(x,x_2)} \geq \frac{1}{d_G(x,z_1)}$. In addition, it is easy to see that $\sum_{y \in S_3} \frac{1}{d_H(y,x_2)} > \sum_{y \in S_3} \frac{1}{d_G(y,z_1)}$. So, we have $k(D_H(x_2) - D_G(z_1)) > 0$.

Thus, we proved that

$$d_H(z_1)D_H(z_1) + d_H(x_2)D_H(x_2) > d_G(z_1)D_G(z_1) + d_G(x_2)D_G(x_2).$$

In view of (1) – (3), we obtain $RDD(G) < RDD(H)$. ■

REMARK 3.2. *The graphs G and H in Lemma* 3.1 *possess the same number of cut vertices. Moreover, If taking $s = 1$ in Lemma* 3.1, *the edge uv of G will become a pendent edge of H.*

If taking $G_2 = x_1 \dots x_t$ in Lemma 3.1, we will get the following result.

COROLLARY 3.3. *Let G be a connected graph. $uv \in E(G)$ and $N_G(u)\backslash\{v\} = N_G(v)\backslash\{u\} \neq \emptyset$. Let $G_{s,t}$ be obtained from G by attaching a path P_t at u and a path P_s at v. If $t \geq s+2 \geq 3$, then $RDD(G_{t,s}) < RDD(G_{t-1,s+1})$.*

LEMMA 3.4. *Let K_puK_q be the union of two complete graphs K_p and K_q sharing exactly one common vertex u, where $p \geq 3, q \geq 3$. Let G be obtained from K_puK_q by attaching a path P_t at some vertex $w_1 \in V(K_p)\backslash\{u\}$ and a path P_s at some vertex $v_1 \in V(K_q)\backslash\{u\}$, and possibly attaching some connected graphs at other vertices of $V(K_puK_q)\backslash\{u, v_1, w_1\}$, where $t \geq s \geq 1$, and let H be obtained from G by deleting the edges of K_q incident to v_1 except v_1u and adding all possible edges between each of $V(K_q)\backslash\{v_1\}$ and each of $V(K_p)$, where G and H are shown in Fig.* 3.2. *Then $RRD(G) < RRD(H)$.*

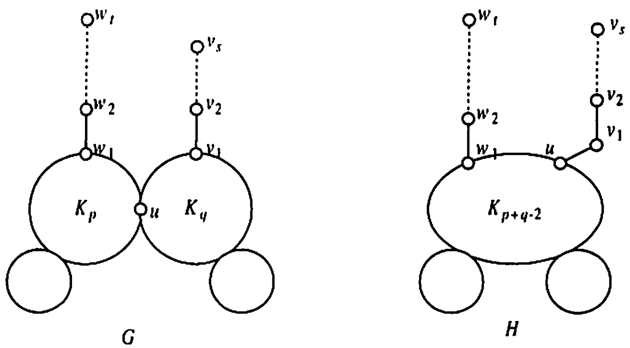

Fig. 3.2 The graphs G and H in Lemma 3.4.

Proof: If $t > s$, by Lemma 2.1 and Lemma 3.1, the result follows immediately. In what follows, we discuss the case when $s = t$.

Let $S_1 = \{v_1, v_2, \ldots, v_s\}, S_2 = \{w_1, w_2, \ldots, w_t\}, S_3 = \{u\}, S_4 = V(K_q)\backslash\{v_1, u\}$, $S_5 = V(K_p)\backslash\{w_1, u\}$, S_6 be the vertex set of the connected graphs attached at the vertices of $V(K_q)\backslash\{u, v_1\}$, excluding the attachment points, S_7 be the vertex set of the connected graphs which attached at the vertices of $V(K_p)\backslash\{u, w_1\}$, excluding the attachment points. Then $V(G)$ can be partitioned as $V(G) = \cup_{i=1}^{7} S_i$. Observe the transformation from G to H, the degree of v_1 changes from q to 2, the degree of w_1 changes from p to $p + q - 2$, the degree of any vertex in S_4 is increased by $p - 2$, the degree of any vertex in S_5 is increased by $q - 2$, while the degrees of any other vertex is unchanged; the distance between any vertex of $S_4 \cup S_6$ and any of S_1 are increased by 1, the distance between any vertex of $S_4 \cup S_6$ and any of $S_2 \cup S_5 \cup S_7$ is decreased by 1, while the distance between any other two vertices is not changed.

(1) Firstly, we consider the vertices v_2 and w_2.

$$\begin{aligned} & d_H(v_2)D_H(v_2) - d_G(v_2)D_G(v_2) + d_H(w_2)D_H(w_2) - d_G(w_2)D_G(w_2) \\ = \; & 2\Big(\sum_{x\in S_4\cup S_6} \tfrac{1}{d_G(v_2,x)+1} - \sum_{x\in S_4\cup S_6} \tfrac{1}{d_G(v_2,x)}\Big) + 2\Big(\sum_{x\in S_4\cup S_6} \tfrac{1}{d_G(w_2,x)-1} - \sum_{x\in S_4\cup S_6} \tfrac{1}{d_G(w_2,x)}\Big). \end{aligned}$$

For any vertex $x \in S_4 \cup S_6$, let $d_G(w_2, x) = a$, then $d_G(v_2, x) = a - 1$. So,

$$\Big(\frac{1}{d_G(v_2,x)+1} - \frac{1}{d_G(v_2,x)}\Big) + \Big(\frac{1}{d_G(w_2,x)-1} - \frac{1}{d_G(w_2,x)}\Big) = \frac{1}{a} - \frac{1}{a-1} + \frac{1}{a-1} - \frac{1}{a} = 0.$$

Hence, $d_H(v_2)D_H(v_2) + d_H(w_2)D_H(w_2) - d_G(v_2)D_G(v_2) - d_G(w_2)D_G(w_2) = 0$.

Similarly, for any v_i and w_i, $i = 3, \ldots, s$, $d_G(v_i)D_G(v_i) + d_G(w_i)D_G(w_i) = d_H(v_i)D_H(v_i) + d_H(w_i)D_H(w_i)$.

(2) For the vertex u, $d_G(u) = d_H(u)$, and the distance from u to any other vertex is unchanged, so $d_G(u)D_G(u) = d_H(u)D_H(u)$.

(3) For any vertex $x \in S_4$, the degree of x is increased by $p-2$, the distance from x to any vertex of S_1 is increased by 1, the distance from x to any vertex of $S_2 \cup S_5 \cup S_7$ is decreased by 1. For any $i = 1, 2, \ldots, s$, let $d_G(x, v_i) = a_i$, then $d_G(x, w_i) = a + 1$, so $\frac{1}{d_H(x,v_i)} + \frac{1}{d_H(x,w_i)} - \frac{1}{d_G(x,v_i)} - \frac{1}{d_G(x,w_i)} = \frac{1}{a_i+1} + \frac{1}{a_i} - \frac{1}{a_i} - \frac{1}{a_i+1} = 0$. Hence, $d_G(x)D_G(x) < d_H(x)d_H(x)$.

(4) For any vertex $x \in S_5$, the degree of x is increased by $q-2$, the distance from x to any vertex of $S_4 \cup S_6$ is decreased by 1, and the distance from x to any other vertex is unchanged. Hence, $d_G(x)D_G(x) < d_H(x)D_H(x)$.

(5) For any vertex $x \in S_6$, the degree of x is unchanged, the distance from x to any vertex of S_1 is increased by 1, the distance from x to any vertex of $S_2 \cup S_5 \cup S_7$ is decreased by 1. By similar discussion to the vertex of S_4, we can get $d_G(x)D_G(x) < d_H(x)d_H(x)$.

(6) For any vertex $x \in S_7$, the degree of x is unchanged, the distance from x to any vertex of $S_4 \cup S_6$ is decreased by 1, and the distance from x to any other vertex is unchanged. Hence, $d_G(x)D_G(x) < d_H(x)D_H(x)$.

(7) In the last step, we concentrate on the vertices v_1 and w_1. From G to H, the degree of v_1 is changed from q to 2, the degree of w_1 is changed from p to $p+q-2$, the distance from v_1 to any vertex of $S_4 \cup S_6$ is increased by 1, the distance from v_1 to any other vertex is unchanged, the distance from w_1 to any vertex of $S_4 \cup S_6$ is decreased by 1, the distance from w_1 to any other vertex is unchanged. For simplicity, let $A = S_4 \cup S_6$, $B = V(G) - S_4 \cup S_6$. Thus, we have

$$\begin{aligned} & d_H(v_1)D_H(v_1) - d_G(v_1)D_G(v_1) + d_H(w_1)D_H(w_1) - d_G(w_1)D_G(w_1) \\ = \; & 2\sum_{x\in A} \frac{1}{d_H(v_1,x)} - q\sum_{x\in A} \frac{1}{d_G(v_1,x)} + (p+q-2)\sum_{x\in A} \frac{1}{d_H(w_1,x)} - p\sum_{x\in A} \frac{1}{d_G(w_1,x)} \\ & +(2-q)\sum_{x\in B-\{v_1\}} \frac{1}{d_G(v_1,x)} + (q-2)\sum_{x\in B-\{w_1\}} \frac{1}{d_G(w_1,x)}. \end{aligned}$$

For any $x \in A$, let $d_G(v_1, x) = a$, then $d_G(w_1, x) = a+1$, $d_H(v_1, x) = a+1$, $d_H(w_1, x) = a$, thus,

$$\frac{2}{d_H(v_1,x)} - \frac{q}{d_G(v_1,x)} + \frac{p+q-2}{d_H(w_1,x)} - \frac{p}{d_G(w_1,x)} = \frac{2}{a+1} - \frac{q}{a} + \frac{p+q-2}{a} - \frac{p}{a+1} > 0.$$

Hence,

$$2\sum_{x\in A}\frac{1}{d_H(v_1,x)}-q\sum_{x\in A}\frac{1}{d_G(v_1,x)}+(p+q-2)\sum_{x\in A}\frac{1}{d_H(w_1,x)}-p\sum_{x\in A}\frac{1}{d_G(w_1,x)}>0.$$

In addition, for any vertex pairs v_i and w_i, $(i = 2,3,\ldots,s)$, $\frac{1}{d_G(w_1,v_i)}+\frac{1}{d_G(w_1,w_i)} = \frac{1}{d_G(v_1,v_i)}+\frac{1}{d_G(v_1,w_i)}$; for the vertex u, $d_G(w_1,u) = d_G(v_1,u)$; while for any vertex $x \in S_5 \cup S_7, d_G(w_1,x) < d_G(v_1,x)$. Thus, by a simple calculation, we have

$$(2-q)\sum_{x\in B-\{v_1\}}\frac{1}{d_G(v_1,x)}+(q-2)\sum_{x\in B-\{w_1\}}\frac{1}{d_G(w_1,x)}>0.$$

Therefore,

$$d_H(v_1)D_H(v_1)-d_G(v_1)D_G(v_1)+d_H(w_1)D_H(w_1)-d_G(w_1)D_G(w_1)>0.$$

Combining (1) – (7), the result follows. ■

REMARK 3.5. *The graphs G and H in Lemma 3.4 possess the same number of cut vertices. Moreover, if $s = 1$, the edge uv_1 of G becomes a pendent edge of H.*

THEOREM 3.6. *For any $G \in \mathcal{G}_{n,k}$, where $0 \le k \le n-2$, $RDD(G) \le RDD(G_{n,k})$, with equality holds if and only if $G \cong G_{n,k}$.*

Proof: Let G_0 be a graph with the maximal reciprocal degree distance among all the graphs with n vertices and k cut vertices. If $k = 0$, then by Lemma 2.1, $G_0 \cong K_n \cong G_{n,0}$. Suppose in what follows that $1 \le k \le n-2$.

Claim 1: G_0 is connected.

If G_0 is disconnected, then G_0 has at least two components. Let z be a cut vertex of G_0. Then z is also a cut vertex of some component, say H_1, of G_0. Let H_2 be another component of G_0. If there is a cut vertex, say z', in H_2, then $G_0 + zz'$ possesses k cut vertices, and by Lemma 2.1, $RDD(G_0) < RDD(G_0 + zz')$, a contradiction. If there is no cut vertex in H_2, then denote by G_0' the graph obtained from G_0 by adding the edges between z and all vertices of H_2. Thus G_0' also possesses k cut vertices, and by Lemma 2.1, $RDD(G_0) < RDD(G_0')$, a contradiction again. Hence G_0 is connected.

By Lemma 2.1, each block of G_0 is complete, and each cut vertex of G_0 is contained exactly in two blocks. If each block of G_0 has exactly two vertices, i.e., each block is a single edge, then G_0 is a tree with maximum degree two, i.e.,

$G_0 \cong P_n \cong G_{n,n-2}$. Suppose in what follows that there is at least one block of G_0 with at least three vertices.

Claim 2: If $G_0 \neq G_{n,1}$, then each pendent block of G_0 is an edge.

If B_1 is a pendent block of G_0 and $|V(B_1)| > 2$, we assume u is a vertex different from the unique cut vertex, say w, of B_1. Denote by B_2 the block adjacent to B_1. By deleting the edges between u and $V(B_1) - \{u, w\}$, and adding all the edges between $V(B_1) - \{u, w\}$ and $V(B_2) - w$, we obtain a new graph G_0'. Notice that the number of cut vertices of G_0' is also k, and by remark 3.2 (if $|V(B_2)| = 2$) and remark 3.5 (if $|V(B_2)| > 2$), we have $RDD(G_0) < RDD(G_0')$, a contradiction.

Choose a pendent path, say P_s at v, with minimal length in G_0. Obviously, v lies in some block, say B, of G_0 with at least three vertices. Note that v is not a cut vertex of G_0 if $s = 1$.

Claim 3: The component attached at any vertex of B is a path(possibly being trivial).

For $x \in V(B)$, let $H^{(x)}$ be the component of $G - E(B)$ containing x. Obviously, $H^{(v)} \cong P_s$. Suppose u is an arbitrary vertex of B and $u \neq v$. Obviously, $N_B(v)\backslash\{u\} = N_B(u)\backslash\{v\}$. Let G^* be the component of $G - ((E(H^{(u)}) \cup E(P_s))$ containing u, which surely contains the block B.

Suppose that $H^{(u)}$ is not a (possibly trivial) path. Then $H^{(u)}$ contains a block with at least three vertices. By the proof of Claim 2, $H^{(u)}$ must contain a nontrivial pendant path P_t attached at some nontrivial block B_0 of $H^{(u)}$, where $s \geq t$. Therefore $H^{(u)}$ contains a shortest path P_r from u to the pendent vertex of P_t, where $r \geq t + 1 \geq s + 1$. If $s = 1$, then by Remark 3.2, we may get another graph with n vertex and k cut vertices, which has a larger reciprocal degree distance, a contradiction. If $s > 1$ and $r \geq s + 2$, then by Lemma 3.1, we also get a contradiction. So in what follows we only need to consider the case:$s > 1$ and $r = s + 1$. In this case, B_0 share with B the common vertex u, and $H^{(u)}$ is obtained from B_0 by attaching P_s at each of its vertices except u. Applying Lemma 3.4, we can get another graph of order n with k cut vertices, which has a larger reciprocal degree distance, a contradiction. Therefore $H^{(u)}$ is a pendent path attached at u which contains at least s vertices.

Claim 4: All paths attached at the vertices of B have almost equal lengths.

Obviously, $t \geq s$. If $t \geq s+2$, then by Corollary 3.3, we may get another graph with n vertices and k cut vertices, which has a larger reciprocal degree distance, a contradiction. So $H^{(u)} \cong P_s$ or P_{s+1}.

Consequently, we get $G \cong G_{n,k}$. ∎

4 Maximum reciprocal degree distance of graphs with given number of cut edges

Similar to section 3, we first introduce two edge-grafting transformations to study the mathematical properties of the reciprocal degree distance of G. Then using these mathematical properties, we characterize the extremal graphs with the maximum RDD-value among all the graphs of order n with given number of cut edges. In addition, we also provide an upper bound on the reciprocal degree distance in terms of the number of cut edges. The following lemma is a special case of Theorem 2.1 in [14].

LEMMA 4.1. *Let $w_1w_2 \in E(G)$ be a cut edge in G, and $G - w_1w_2 = G_1 \cup G_2$ where G_i is nontrivial and $w_i \in V(G_i)$ for $i = 1,2$. Assume that H is a graph obtained from G by identifying w_1 with w_2 (the new vertex is labeled as w) and attaching at w a pendent vertex w_0. G and H are shown in Fig. 4.1. Then $RDD(G) < RDD(H)$.*

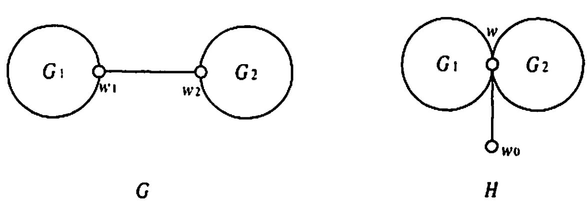

Fig. 4.1 The graphs G and H in Lemma 4.1.

LEMMA 4.2. *Let G_0, G_1, G_2 be pairwise vertex-disjoint connected graphs and $u, v \in V(G_0)$ such that $N_{G_0}(u)\backslash\{v\} = N_{G_0}(v)\backslash\{u\}$, $w_1 \in V(G_1)$, $w_2 \in V(G_2)$. Let H be the graph obtained from G_0, G_1, G_2 by identifying u with w_1 and v with w_2, respectively. Let H_1 be the graph obtained from G_0, G_1, G_2 by identifying three vertices u, w_1, w_2, and let H_2 be the graph obtained from G_0, G_1, G_2 by identifying three vertices v, w_1, w_2. H, H_1 and H_2 are shown in Fig. 4.2. Then we have $RDD(H_i) > RDD(H)$ for $i = 1,2$.*

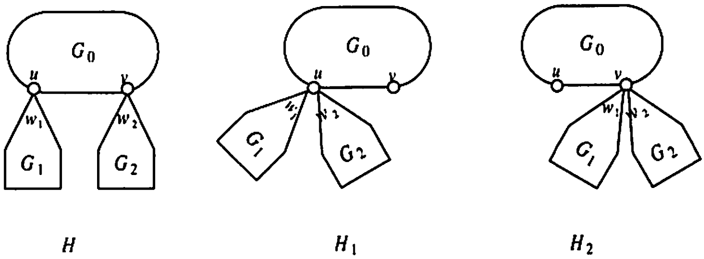

Fig. 4.2 The graphs H, H_1 and H_2 in Lemma 4.2.

Proof: Denote $G_0-\{u,v\}$ by G_0^*, G_1-w_1 by G_1^* and G_2-w_2 by G_2^*, then $V(H) = V(H_1) = V(H_2) = V(G_0^*)\cup V(G_1^*)\cup V(G_2^*)\cup\{u,v\}$. Obviously, $V(G_0^*)$, $V(G_1^*)$, $V(G_2^*)$ and$\{u,v\}$ are four vertex sets disjoint in pair. Since $N_{G_0}(u)\backslash\{v\} = N_{G_0}(v)\backslash\{u\}$, we have $d_{G_0}(u) = d_{G_0}(v)$ and for any $x \in V(G_0^*)$, $d_{G_0}(u,x) = d_{G_0}(v,x)$. Note that from H to $H_i (i = 1,2)$, the vertices which degree changed only are u and v. Also in H, H_1 or H_2, u and v have the same distance. For simplicity, we denote by $d(u,v)$ the distance between u and v in H, H_1 or H_2. Similarly, $d(x,u)$ ($d(x,v)$, respectively) denotes the distance between x and u (v, respectively) for any $x \in V(G_0^*)$, $d(w_1,y)$ denotes the distance between w_1 and y for any $y \in V(G_1^*)$, and $d(w_2,z)$ denotes the distance between w_2 and z for any $z \in V(G_2^*)$. Therefore,

$$
\begin{aligned}
&RDD(H_1) - RDD(H) \\
&= \sum_{x\in V(G_0^*)} [d(x) \sum_{z\in V(G_2^*)} (\tfrac{1}{d_{H_1}(x,z)} - \tfrac{1}{d_H(x,z)})] + \sum_{y\in V(G_1^*)} [d(y) \sum_{z\in V(G_2^*)} (\tfrac{1}{d_{H_1}(y,z)} - \tfrac{1}{d_H(y,z)})] \\
&+ \sum_{z\in V(G_2^*)} [d(z)(\sum_{x\in V(G_0^*)} (\tfrac{1}{d_{H_1}(x,z)} - \tfrac{1}{d_H(x,z)}) + \sum_{y\in V(G_1^*)} (\tfrac{1}{d_{H_1}(y,z)} - \tfrac{1}{d_H(y,z)}) + \tfrac{1}{d_{H_1}(z,u)} - \tfrac{1}{d_H(z,u)} \\
&+ \tfrac{1}{d_{H_1}(z,v)} - \tfrac{1}{d_H(z,v)})] + d_{H_1}(u)(\sum_{x\in V(G_0^*)} \tfrac{1}{d(x,u)} + \sum_{y\in V(G_1^*)} \tfrac{1}{d(w_1,y)} + \sum_{z\in V(G_2^*)} \tfrac{1}{d(w_2,z)} + \tfrac{1}{d(u,v)}) \\
&- d_H(u)(\sum_{x\in V(G_0^*)} \tfrac{1}{d(x,u)} + \sum_{y\in V(G_1^*)} \tfrac{1}{d(w_1,y)} + \sum_{z\in V(G_2^*)} \tfrac{1}{d(u,v)+d(w_2,z)} + \tfrac{1}{d(u,v)}) \\
&+ d_{H_1}(v)(\sum_{x\in V(G_0^*)} \tfrac{1}{d(x,v)} + \sum_{y\in V(G_1^*)} \tfrac{1}{d(w_1,y)+d(u,v)} + \sum_{z\in V(G_2^*)} \tfrac{1}{d(w_2,z)+d(u,v)} + \tfrac{1}{d(u,v)}) \\
&- d_H(v)(\sum_{x\in V(G_0^*)} \tfrac{1}{d(x,v)} + \sum_{y\in V(G_1^*)} \tfrac{1}{d(w_1,y)+d(u,v)} + \sum_{z\in V(G_2^*)} \tfrac{1}{d(w_2,z)} + \tfrac{1}{d(u,v)}) \\
&> (d_{G_0}(u) + d_{G_1}(w_1) - d_{G_0}(v)) \sum_{z\in V(G_2^*)} (\tfrac{1}{d(w_2,z)} - \tfrac{1}{d(u,v)+d(w_2,z)}) + d_{G_2}(w_2) \sum_{x\in V(G_0^*)} (\tfrac{1}{d(x,u)} \\
&- \tfrac{1}{d(x,v)}) + \sum_{x\in V(G_0^*)} \sum_{z\in V(G_2^*)} (d(x) + d(z))(\tfrac{1}{d(x,u)+d(w_2,z)} - \tfrac{1}{d(x,v)+d(w_2,z)}) \\
&= d_{G_1}(w_1) \sum_{z\in V(G_2^*)} (\tfrac{1}{d(w_2,z)} - \tfrac{1}{d(u,v)+d(w_2,z)}) \\
&> 0.
\end{aligned}
$$

Similarly, we have $RDD(H_2) - RDD(H) > 0$. The result follows. ■

THEOREM 4.3. *For any $G \in \overline{\mathcal{G}}_{n,k}$, where $0 \le k \le n-1$,*

(1) *if $k = n-2$, then*

$$RDD(G) \le \frac{3}{2}n^2 - \frac{11}{2}n + 5,$$

with equality holds if and only if $G \cong S_{n-1} \cup K_1$.

(2) *if $k \ne n-2$, then*

$$RDD(G) \le n^3 - (\frac{5}{2}k + 2)n^2 + (2k^2 + \frac{11}{2}k + 1)n - (\frac{1}{2}k^3 + 2k^2 + \frac{5}{2}k),$$

with equality holds if and only if $G \cong \overline{G}_{n,k}$.

Proof: Let G_0 be a graph with the maximum reciprocal degree distance in $\overline{\mathcal{G}}_{n,k}$ and $E_1 = \{e_1, e_2, \ldots, e_k\}$ be the set of cut edges of G_0.

If $k = 0$, then by Lemma 2.1, $G_0 \cong K_n \cong \overline{G}_{n,0}$.

If $k = n-1$, then G_0 must be a tree. By Lemma 4.1, we can easily get $G_0 \cong S_n \cong \overline{G}_{n,n-1}$.

If $k = n-2$, then G_0 must be the union of two trees. By Lemma 4.1, the two trees are both stars, say S_m and S_{n-m}, where $1 \le m \le n-1$. By a simple calculation, we can get $RDD(S_m \cup S_{n-m}) = 3m^2 - 3nm + \frac{3}{2}n^2 - \frac{5}{2}n + 2$. Hence, when $m = 1$ or $m = n-1$, $RDD(S_m \cup S_{n-m})$ gets the maximum value, that is $\frac{3}{2}n^2 - \frac{11}{2}n + 5$. In this case, $G_0 \cong S_{n-1} \cup K_1$.

Suppose in what follows that $1 \le k \le n-3$.

Firstly, by Lemma 2.1, we can get that each component of $G_0 - E_1$ is a clique.

In addition, we can get that G_0 is connected. Assume G_0 that is disconnected. If G_0 is a forest, then G_0 has at least three components. And by Lemma 4.1, each component is a star. Then denote by G_0' the graph obtained from G_0 by adding the edges between all centers of these components. Thus G_0' possesses k cut edges, and by Lemma 2.1, $RDD(G_0) < RDD(G_0')$, a contradiction. If G_0 is not a forest,then G_0 has at least two components and there exists a clique which contains at least three vertices in some component. Let H_1, H_2 be two components of G_0, and Q_1(Q_2,respectively) be a clique of H_1(H_2,respectively), where Q_1 contains at least three vertices. Then denote by G_0' the graph obtained from G_0 by adding the edges between all vertices of Q_1 and all vertices of Q_2. Thus G_0' also possesses k cut edges, and by Lemma 2.1, $RDD(G_0) < RDD(G_0')$, another contradiction. Hence G_0 is connected.

Moreover, by Lemma 4.1, $e_1, e_2, \ldots, e_k$ must be the pendent edges in G_0. Hence, G_0 must be the graph obtained from K_{n-k} by attaching k pendent edges to some vertices.

Finally, by Lemma 4.2, all these pendent edges in G_0 must be attached to one common vertex. Thus $G_0 \cong \overline{G}_{n,k}$.

So we only need to calculate $RRD(\overline{G}_{n,k})$. By the structure of $\overline{G}_{n,k}$, we get

$$\begin{aligned} RDD(\overline{G}_{n,k}) &= k(1+\tfrac{n-2}{2}) + (n-1)^2 + (n-k-1)\left[(n-k-1)(n-k-1+\tfrac{k}{2})\right] \\ &= n^3 - (\tfrac{5}{2}k+2)n^2 + (2k^2+\tfrac{11}{2}k+1)n - (\tfrac{1}{2}k^3+2k^2+\tfrac{5}{2}k). \end{aligned}$$

This completes the proof. ■

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