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General degree distance of graphs

Research Article

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Abstract: We generalize several topological indices and introduce the general degree distance of a connected graph G. For $a, b \in \mathbb{R}$, the general degree distance $DD_{a,b}(G) = \sum_{v \in V(G)} [deg_G(v)]^a S_G^b(v)$, where $V(G)$ is the vertex set of G, $deg_G(v)$ is the degree of a vertex v, $S_G^b(v) = \sum_{w \in V(G) \setminus \{v\}} [d_G(v, w)]^b$ and $d_G(v, w)$ is the distance between v and w in G. We present some sharp bounds on the general degree distance for multipartite graphs and trees of given order, graphs of given order and chromatic number, graphs of given order and vertex connectivity, and graphs of given order and number of pendant vertices.

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1. Introduction

We denote the vertex set and edge set of a graph G by $V(G)$ and $E(G)$, respectively The number of vertices of G is called the order. For $v \in V(G)$, the degree of v, $deg_G(v)$, is the number of vertices adjacent to v. The distance between two vertices v and w in G, denoted by $d_G(v, w)$, is the number of edges in a shortest path between v and w. We denote the complete graph and the star of order n by K_n and S_n, respectively.

Topological indices are molecular descriptors which have been studied due to their extensive applications. These graph invariants play an important role in engineering, materials science, pharmaceutical sciences and especially in chemistry, since they can be correlated with many chemical and physical properties of molecules. Graph theory can be used to characterize these chemical structures.

One of the most well-known distance-based topological indices is the degree distance. The degree distance of a connected graph G,

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

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was introduced independently by Dobrynin and Kochetova [5] and Gutman [6]. Bounds on the degree distance for graphs with given vertex connectivity were obtained in [2], bounds for graphs with given edge connectivity in [1], bounds for graphs of minimum degree in [13], bounds for cacti in [20] and bounds for bicyclic graphs in [3]. The degree distance for unicyclic graphs with prescribed matching number was investigated in [10] and graph products were studied in [19] and [16]. Relations between the degree distance and the eccentric distance sum were investigated in [9] and relations between the degree distance and the Gutman index in [4].

The reciprocal degree distance

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

of a connected graph G has been widely studied too. Bounds on the reciprocal degree distance for graphs with cut edges or cut vertices were given in [12], bounds for bipartite graphs and outerplanar graphs in [11]. The reciprocal degree distance of graph products was studied in [15] and the Steiner reciprocal degree distance in [17]. The generalized degree distance was first presented in [8] and studied for example in [7] and [14].

For $a, b \in \mathbb{R}$, we introduce the general degree distance of a connected graph G as

$$\begin{aligned} DD_{a,b}(G) &= \sum_{v \in V(G)} \Big([deg_G(v)]^a \sum_{w \in V(G) \setminus \{v\}} [d_G(v,w)]^b \Big) \\ &= \sum_{\{v,w\} \subseteq V(G)} ([deg_G(v)]^a + [deg_G(w)]^a) [d_G(v,w)]^b. \end{aligned}$$

Let $S_G^b(v) = \sum_{w \in V(G) \setminus \{v\}} [d_G(v,w)]^b$. Then we can write

$$DD_{a,b}(G) = \sum_{v \in V(G)} [deg_G(v)]^a S_G^b(v).$$

If $a = 1$, then $DD_{1,b}(G)$ is the generalized degree distance. If $a = 1$ and $b = 1$, we get the classical degree distance. If $a = 1$ and $b = -1$, we get the reciprocal degree distance. If $a = 0$ and $b = 1$, then $DD_{0,1}(G) = 2W(G)$, where $W(G)$ is the Wiener index. If $a = 0$ and $b = -1$, then $DD_{0,-1}(G) = 2H(G)$, where $H(G)$ is the Harary index. We present several bounds on the general degree distance of graphs.

2. Preliminary results

Lemmas 2.1 and 2.2 are used in the proofs of some main results. Note that $(a,b) \neq (0,0)$ means that not both a and b are 0.

Lemma 2.1. *Let G be any connected graph such that u_1 and u_2 are non-adjacent vertices in G. Then for $a \leq 0$ and $b \geq 0$, where $(a,b) \neq (0,0)$,*

$$DD_{a,b}(G + u_1u_2) < DD_{a,b}(G).$$

Proof. Let G' be the graph $G + u_1u_2$. Then for any two vertices $v, w \in V(G)$, we get $d_{G'}(v,w) \leq d_G(v,w)$ and $[d_{G'}(v,w)]^b \leq [d_G(v,w)]^b$, where $b \geq 0$. Therefore, $S_{G'}^b(v) \leq S_G^b(v)$ for each $v \in V(G)$, where $b \geq 0$. For $v \in V(G) \setminus \{u_1, u_2\}$, we have $deg_{G'}(v) = deg_G(v)$, thus $[deg_{G'}(v)]^a = [deg_G(v)]^a$ and $[deg_{G'}(v)]^a S_{G'}^b(v) \leq [deg_G(v)]^a S_G^b(v)$ for $a \leq 0$ and $b \geq 0$.

Now we consider the vertices u_1 and u_2. Since $1 = d_{G'}(u_1,u_2) < d_G(u_1,u_2)$, we obtain $[d_{G'}(u_1,u_2)]^b < [d_G(u_1,u_2)]^b$ for $b > 0$. Thus $S_{G'}^b(u_i) < S_G^b(u_i)$ for $i = 1, 2$. Note that if $b = 0$, then $S_{G'}^b(u_i) = S_G^b(u_i)$.

For the degrees, we have $deg_{G'}(u_i) = deg_G(u_i) + 1$. For $a < 0$, we obtain $[deg_{G'}(u_i)]^a < [deg_G(u_i)]^a$, and for $a = 0$, we have $[deg_{G'}(u_i)]^a = [deg_G(u_i)]^a = 1$. It follows that $[deg_{G'}(u_i)]^a \ S^b_{G'}(u_i) < [deg_G(u_i)]^a S^b_G(u_i)$ for $a \leq 0$ and $b \geq 0$, where $(a, b) \neq (0, 0)$. Thus

$$\begin{aligned} DD_{a,b}(G') &= \sum_{i=1}^{2}[deg_{G'}(u_i)]^a S^b_{G'}(u_i) + \sum_{v \in V(G') \setminus \{u_1,u_2\}} [deg_{G'}(v)]^a S^b_{G'}(v) \\ &< \sum_{i=1}^{2}[deg_{G}(u_i)]^a S^b_{G}(u_i) + \sum_{v \in V(G) \setminus \{u_1,u_2\}} [deg_{G}(v)]^a S^b_{G}(v) \\ &= DD_{a,b}(G'). \end{aligned}$$

□

Lemma 2.2. *Let G be any connected graph such that u_1 and u_2 are non-adjacent vertices in G. Then for $a \geq 0$ and $b \leq 0$, where $(a, b) \neq (0, 0)$,*

$$DD_{a,b}(G + u_1u_2) > DD_{a,b}(G).$$

Proof. Let G' be the graph $G + u_1u_2$. Then for any two vertices $v, w \in V(G)$, we get $d_{G'}(v, w) \leq d_G(v, w)$ and $[d_{G'}(v, w)]^b \geq [d_G(v, w)]^b$, where $b \leq 0$. Therefore, $S^b_{G'}(v) \geq S^b_G(v)$ for each $v \in V(G)$, where $b \leq 0$. For $v \in V(G) \setminus \{u_1, u_2\}$, we have $deg_{G'}(v) = deg_G(v)$, thus $[deg_{G'}(v)]^a = [deg_G(v)]^a$ and $[deg_{G'}(v)]^a S^b_{G'}(v) \geq [deg_G(v)]^a S^b_G(v)$ for $a \geq 0$ and $b \leq 0$.

Now we consider the vertices u_1 and u_2. Since $1 = d_{G'}(u_1, u_2) < d_G(u_1, u_2)$, we obtain $1 = [d_{G'}(u_1, u_2)]^b > [d_G(u_1, u_2)]^b > 0$ for $b < 0$. Thus $S^b_{G'}(u_i) > S^b_G(u_i)$ for $i = 1, 2$. Note that if $b = 0$, then $S^b_{G'}(u_i) = S^b_G(u_i)$.

For the degrees, we have $deg_{G'}(u_i) = deg_G(u_i) + 1$. For $a > 0$, we obtain $[deg_{G'}(u_i)]^a > [deg_G(u_i)]^a$, and for $a = 0$, we have $[deg_{G'}(u_i)]^a = [deg_G(u_i)]^a = 1$. It follows that $[deg_{G'}(u_i)]^a \ S^b_{G'}(u_i) > [deg_G(u_i)]^a S^b_G(u_i)$ for $a \geq 0$ and $b \leq 0$, where $(a, b) \neq (0, 0)$. Thus

$$\begin{aligned} DD_{a,b}(G') &= \sum_{i=1}^{2}[deg_{G'}(u_i)]^a S^b_{G'}(u_i) + \sum_{v \in V(G') \setminus \{u_1,u_2\}} [deg_{G'}(v)]^a S^b_{G'}(v) \\ &> \sum_{i=1}^{2}[deg_{G}(u_i)]^a S^b_{G}(u_i) + \sum_{v \in V(G) \setminus \{u_1,u_2\}} [deg_{G}(v)]^a S^b_{G}(v) \\ &= DD_{a,b}(G'). \end{aligned}$$

The proof is complete. □

Lemma 2.3 was presented in [18]. We use it in the next section to compare the $DD_{a,b}$ indices of some graphs.

Lemma 2.3. *Let $1 \leq x < y$ and $c > 0$. For $a > 1$ and $a < 0$, we have*

$$(x + c)^a - x^a < (y + c)^a - y^a.$$

3. Main results

From Lemma 2.1, we know that among graphs of order n, the complete graph K_n is the graph having the smallest general degree distance for $a \leq 0$ and $b \geq 0$, where $(a, b) \neq (0, 0)$. Similarly, by Lemma 2.2, among graphs of order n, K_n is the graph having the largest general degree distance for $a \geq 0$ and $b \leq 0$, where $(a, b) \neq (0, 0)$.

For an integer $k \geq 2$, a k-partite graph is a graph such that we can divide its vertices into k disjoint sets, where any vertices in the same set are non-adjacent. A 2-partite graph is called a bipartite graph. The complete k-partite graph with partite sets of orders $n_1, n_2, \ldots, n_k$ is denoted by $K_{n_1,n_2,\ldots,n_k}$. Any two vertices which are not in the same partite set of $K_{n_1,n_2,\ldots,n_k}$ are adjacent. If n_i and n_j differ by at most 1 for every i, j, where $1 \leq i < j \leq k$, then the graph $K_{n_1,n_2,\ldots,n_k}$ of order n is called the Turán graph and it is denoted by $T(n, k)$. We show that $T(n, k)$ has the smallest $DD_{a,b}$ index among k-partite graphs with n vertices.

Theorem 3.1. *Let G be any k-partite graph of order n, where $2 \leq k \leq n$. Then for $a \leq 0$ and $b \geq 0$, where $(a, b) \neq (0, 0)$, we have*

$$DD_{a,b}(G) \geq DD_{a,b}(T(n, k))$$

with equality only if G is the Turán graph $T(n, k)$.

Proof. Let G' be a graph having the smallest $DD_{a,b}$ index among k-partite graphs of order n. By Lemma 2.1, any two vertices in different partite sets must be adjacent. Thus G' is $K_{n_1,n_2,\ldots,n_k}$ for some positive integers $n_1, n_2, \ldots, n_k$. We prove by contradiction that n_i and n_j differ by at most 1 for every i, j, where $1 \leq i < j \leq k$.

Assume that n_i and n_j differ by at least 2 for some i, j, where $1 \leq i < j \leq k$. Without loss of generality, assume that $n_1 \geq n_2 + 2$. We compare the $DD_{a,b}$ indices of $G' = K_{n_1,n_2,\ldots,n_k}$ and $G'' = K_{n_1-1,n_2+1,\ldots,n_k}$.

For every vertex v from the first partite set and v' from the second partite set of $K_{n_1,n_2,\ldots,n_k}$, we have

$$deg_{G'}(v) = n - n_1, \quad S^b_{G'}(v) = 1^b(n - n_1) + 2^b(n_1 - 1)$$

and

$$deg_{G'}(v') = n - n_2, \quad S^b_{G'}(v') = 1^b(n - n_2) + 2^b(n_2 - 1).$$

For every vertex w from the first partite set and w' from the second partite set of $K_{n_1-1,n_2+1,\ldots,n_k}$, we have

$$deg_{G''}(w) = n - (n_1 - 1), \quad S^b_{G''}(w) = 1^b(n - (n_1 - 1)) + 2^b(n_1 - 2)$$

and

$$deg_{G''}(w') = n - (n_2 + 1), \quad S^b_{G''}(w') = 1^b(n - (n_2 + 1)) + 2^b n_2.$$

For any other vertex z, we have $deg_{G'}(z) = deg_{G''}(z)$ and $S^b_{G'}(z) = S^b_{G''}(z)$. For $b > 0$,

$$\begin{aligned} S^b_{G'}(v) - S^b_{G''}(w) &= 2^b - 1 > 0, \\ S^b_{G''}(w) - S^b_{G''}(w') &= 2^b(n_1 - n_2 - 2) - n_1 + n_2 + 2 = (2^b - 1)(n_1 - n_2 - 2) \geq 0, \\ S^b_{G''}(w') - S^b_{G'}(v') &= 2^b - 1 > 0, \end{aligned}$$

therefore

$$0 < S^b_{G'}(v') < S^b_{G''}(w') \leq S^b_{G''}(w) < S^b_{G'}(v).$$

For $b = 0$, we obtain $S^b_{G'}(v') = S^b_{G''}(w') = S^b_{G''}(w) = S^b_{G'}(v) = n - 1$. Since $n_1 - 1 \geq n_2 + 1$, we have

$$0 < (n - n_2)^a < (n - n_2 - 1)^a \leq (n - n_1 + 1)^a < (n - n_1)^a$$

for $a < 0$. Obviously, for $a = 0$, we get $(n-n_2)^a = (n-n_2-1)^a = (n-n_1+1)^a = (n-n_1)^a = 1$. Thus, for $a \le 0$ and $b \ge 0$, where $(a,b) \ne (0,0)$, we have

$$\begin{aligned}
DD_{a,b}(G') - DD_{a,b}(G'') &= n_1(n-n_1)^a S^b_{G'}(v) + n_2(n-n_2)^a S^b_{G'}(v') \\
&\quad - (n_1-1)(n-n_1+1)^a S^b_{G''}(w) - (n_2+1)(n-n_2-1)^a S^b_{G''}(w') \\
&= (n_1-1)(n-n_1)^a S^b_{G'}(v) + (n_2+1)(n-n_2)^a S^b_{G'}(v') \\
&\quad + (n-n_1)^a S^b_{G'}(v) - (n-n_2)^a S^b_{G'}(v') \\
&\quad - (n_1-1)(n-n_1+1)^a S^b_{G''}(w) - (n_2+1)(n-n_2-1)^a S^b_{G''}(w') \\
&> (n_1-1)(n-n_1)^a S^b_{G'}(v) + (n_2+1)(n-n_2)^a S^b_{G'}(v') \\
&\quad - (n_1-1)(n-n_1+1)^a S^b_{G''}(w) - (n_2+1)(n-n_2-1)^a S^b_{G''}(w') \\
&= (n_1-1)(n-n_1)^a S^b_{G''}(w) + (n_2+1)(n-n_2)^a S^b_{G''}(w') \\
&\quad + (n_1-1)(n-n_1)^a [S^b_{G'}(v) - S^b_{G''}(w)] \\
&\quad - (n_2+1)(n-n_2)^a [S^b_{G''}(w') - S^b_{G'}(v')] \\
&\quad - (n_1-1)(n-n_1+1)^a S^b_{G''}(w) - (n_2+1)(n-n_2-1)^a S^b_{G''}(w') \\
&\ge (n_1-1)(n-n_1)^a S^b_{G''}(w) + (n_2+1)(n-n_2)^a S^b_{G''}(w') \\
&\quad - (n_1-1)(n-n_1+1)^a S^b_{G''}(w) - (n_2+1)(n-n_2-1)^a S^b_{G''}(w') \\
&= (n_1-1)S^b_{G''}(w)[(n-n_1)^a - (n-n_1+1)^a] \\
&\quad + (n_2+1)S^b_{G''}(w')[(n-n_2)^a - (n-n_2-1)^a] \\
&\ge (n_2+1)S^b_{G''}(w')[(n-n_1)^a - (n-n_1+1)^a] \\
&\quad + (n_2+1)S^b_{G''}(w')[(n-n_2)^a - (n-n_2-1)^a] \\
&\ge 0,
\end{aligned}$$

since for $a = 0$, we obtain $(n-n_1)^a - (n-n_1+1)^a = 0$ and $(n-n_2)^a - (n-n_2-1)^a = 0$, and for $a < 0$, by Lemma 2.3,

$$(n-n_2)^a - (n-n_2-1)^a > (n-n_1+1)^a - (n-n_1)^a,$$

thus

$$(n-n_2)^a - (n-n_2-1)^a + (n-n_1)^a - (n-n_1+1)^a > 0.$$

Hence $DD_{a,b}(G') - DD_{a,b}(G'') > 0$ and $DD_{a,b}(G') > DD_{a,b}(G'')$. So G' is not a graph with the smallest $DD_{a,b}$ index and we have a contradiction. Therefore, n_i and n_j differ by at most 1 which means that G' is the Turán graph $T(n,k)$. □

We can use $k = 2$ in Theorem 3.1 to get the following corollary for bipartite graphs.

Corollary 3.2. *Let G be any bipartite graph of order n, where $n \ge 2$. Then for $a \le 0$ and $b \ge 0$, where $(a,b) \ne (0,0)$, we have*

$$DD_{a,b}(G) \ge DD_{a,b}(K_{\lceil \frac{n}{2} \rceil, \lfloor \frac{n}{2} \rfloor})$$

with equality only if G is $K_{\lceil \frac{n}{2} \rceil, \lfloor \frac{n}{2} \rfloor}$.

The chromatic number of a graph G is the minimum number of colors needed to color the vertices of G so that no two adjacent vertices have the same color. Let us present a bound on the general degree distance for graphs with given chromatic number.

Theorem 3.3. *Let G be any connected graph of order n and chromatic number χ, where $2 \le \chi \le n$. Then for $a \le 0$ and $b \ge 0$, where $(a,b) \ne (0,0)$, we have*

$$DD_{a,b}(G) \ge DD_{a,b}(T(n,\chi))$$

with equality only if G is the Turán graph $T(n,\chi)$.

Proof. Let G' be any graph having the smallest $DD_{a,b}$ index in terms of order n and chromatic number χ. There is no edge between the vertices in the same color class, therefore G' must be a χ-partite graph. Then, by Theorem 3.1, G' is $T(n, \chi)$. □

The union $H = H_1 \cup H_2$ and join $F = H_1 + H_2$ of the graphs H_1 and H_2 have the vertex sets $V(H) = V(F) = V(H_1) \cup V(H_2)$. The edge set $E(H) = E(H_1) \cup E(H_2)$. The set $E(F)$ contains the edges in $E(H)$ and the edges connecting each vertex in $V(H_1)$ and each vertex in $V(H_2)$. We show that $(K_{n-\kappa-1} \cup K_1) + K_\kappa$ has the extremal $DD_{a,b}(G)$ index for graphs of given vertex connectivity, where $a \geq 1$ and $b \leq 0$. The vertex connectivity of G is the minimum number of vertices whose removal disconnects G.

Theorem 3.4. *Let G be any connected graph of order n and vertex connectivity κ, where $1 \leq \kappa \leq n-2$. Then for $a \geq 1$ and $b \leq 0$,*

$$DD_{a,b}(G) \leq DD_{a,b}((K_{n-\kappa-1} \cup K_1) + K_\kappa)$$

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

Proof. Let G' be any graph with the largest $DD_{a,b}$ index with respect to order n and vertex connectivity κ. So there is a set $A \subset V(G')$ of cardinality κ, such that $G' - A$ is disconnected (where $G' - A$ is obtained from G' be the removal of the vertices in A and the removal of each edge of G' incident with a vertex in A). We can divide the vertices in $V(G') \setminus A$ into the sets A_1 and A_2, where no vertex in A_1 is adjacent to a vertex in A_2. By Lemma 2.2, there is an edge connecting each pair of vertices in A_1, each pair of vertices in A_2 and the degree of each vertex in A is $n-1$ in G'.

Let $|A_1| = n_1$ and $|A_2| = n_2$. Without loss of generality, assume that $n_1 \geq n_2 \geq 1$. We get $n - \kappa = n_1 + n_2$ and G' is $(K_{n_1} \cup K_{n_2}) + K_\kappa$. We prove that $n_2 = 1$.

Assume to the contrary that $n_2 \geq 2$ (where $n_1 \geq n_2$). We compare the $DD_{a,b}$ indices of $G' = (K_{n_1} \cup K_{n_2}) + K_\kappa$ and $G'' = (K_{n_1+1} \cup K_{n_2-1}) + K_\kappa$.

For each $z \in A$, we get $deg_{G'}(z) = deg_{G''}(z) = n-1$ and $S^b_{G'}(z) = S^b_{G''}(z) = n-1$. For each $v \in V(K_{n_1})$,

$$deg_{G'}(v) = \kappa + n_1 - 1 \quad \text{and} \quad S^b_{G'}(v) = 1^b(\kappa + n_1 - 1) + 2^b n_2.$$

For each $v' \in V(K_{n_2})$, we obtain

$$deg_{G'}(v') = \kappa + n_2 - 1 \quad \text{and} \quad S^b_{G'}(v') = 1^b(\kappa + n_2 - 1) + 2^b n_1.$$

For each $w \in V(K_{n_1+1})$, we have

$$deg_{G''}(w) = \kappa + n_1 \quad \text{and} \quad S^b_{G''}(w) = 1^b(\kappa + n_1) + 2^b(n_2 - 1).$$

For each $w' \in V(K_{n_2-1})$, we get

$$deg_{G''}(w') = \kappa + n_2 - 2, \quad \text{and} \quad S^b_{G''}(w') = 1^b(\kappa + n_2 - 2) + 2^b(n_1 + 1).$$

For $b \leq 0$,

$$\begin{aligned} S^b_{G''}(w') - S^b_{G'}(v') &= 2^b - 1 \leq 0, \\ S^b_{G'}(v') - S^b_{G'}(v) &= 2^b(n_1 - n_2) - n_1 + n_2 = (2^b - 1)(n_1 - n_2) \leq 0, \\ S^b_{G'}(v) - S^b_{G''}(w) &= 2^b - 1 \leq 0, \end{aligned}$$

therefore

$$0 < S^b_{G''}(w') \leq S^b_{G'}(v') \leq S^b_{G'}(v) \leq S^b_{G''}(w).$$

Note that

$$0 < (\kappa + n_2 - 2)^a < (\kappa + n_2 - 1)^a \leq (\kappa + n_1 - 1)^a < (\kappa + n_1)^a.$$

for $a \geq 1$. Thus for $a \geq 1$ and $b \leq 0$, we have

$$\begin{aligned}
DD_{a,b}(G') - DD_{a,b}(G'') &= n_1(\kappa + n_1 - 1)^a S^b_{G'}(v) + n_2(\kappa + n_2 - 1)^a S^b_{G'}(v') \\
&\quad - (n_1 + 1)(\kappa + n_1)^a S^b_{G''}(w) - (n_2 - 1)(\kappa + n_2 - 2)^a S^b_{G''}(w') \\
&= n_1(\kappa + n_1 - 1)^a S^b_{G'}(v) + n_2(\kappa + n_2 - 1)^a S^b_{G'}(v') \\
&\quad - n_1(\kappa + n_1)^a S^b_{G''}(w) - n_2(\kappa + n_2 - 2)^a S^b_{G''}(w') \\
&\quad - (\kappa + n_1)^a S^b_{G''}(w) + (\kappa + n_2 - 2)^a S^b_{G''}(w') \\
&< n_1(\kappa + n_1 - 1)^a S^b_{G'}(v) + n_2(\kappa + n_2 - 1)^a S^b_{G'}(v') \\
&\quad - n_1(\kappa + n_1)^a S^b_{G''}(w) - n_2(\kappa + n_2 - 2)^a S^b_{G''}(w') \\
&= n_1(\kappa + n_1 - 1)^a S^b_{G'}(v) + n_2(\kappa + n_2 - 1)^a S^b_{G'}(v') \\
&\quad - n_1(\kappa + n_1)^a S^b_{G'}(v) - n_2(\kappa + n_2 - 2)^a S^b_{G'}(v') \\
&\quad - n_1(\kappa + n_1)^a [S^b_{G''}(w) - S^b_{G'}(v)] + n_2(\kappa + n_2 - 2)^a [S^b_{G'}(v') - S^b_{G''}(w')] \\
&\leq n_1(\kappa + n_1 - 1)^a S^b_{G'}(v) + n_2(\kappa + n_2 - 1)^a S^b_{G'}(v') \\
&\quad - n_1(\kappa + n_1)^a S^b_{G'}(v) - n_2(\kappa + n_2 - 2)^a S^b_{G'}(v') \\
&= n_1 S^b_{G'}(v)[(\kappa + n_1 - 1)^a - (\kappa + n_1)^a] \\
&\quad + n_2 S^b_{G'}(v')[(\kappa + n_2 - 1)^a - (\kappa + n_2 - 2)^a] \\
&\leq n_1 S^b_{G'}(v)[(\kappa + n_1 - 1)^a - (\kappa + n_1)^a] \\
&\quad + n_1 S^b_{G'}(v)[(\kappa + n_2 - 1)^a - (\kappa + n_2 - 2)^a] \\
&\leq 0,
\end{aligned}$$

since for $a = 1$, we obtain $(\kappa + n_1 - 1)^a - (\kappa + n_1)^a + (\kappa + n_2 - 1)^a - (\kappa + n_2 - 2)^a = 0$ and for $a > 1$, by Lemma 2.3,

$$(\kappa + n_2 - 1)^a - (\kappa + n_2 - 2)^a < (\kappa + n_1)^a - (\kappa + n_1 - 1)^a,$$

thus

$$(\kappa + n_1 - 1)^a - (\kappa + n_1)^a + (\kappa + n_2 - 1)^a - (\kappa + n_2 - 2)^a < 0.$$

Hence $DD_{a,b}(G') - DD_{a,b}(G'') < 0$ and $DD_{a,b}(G') < DD_{a,b}(G'')$. So G' is not a graph with the largest $DD_{a,b}$ index and we have a contradiction.

We obtain $n_2 = 1$ and consequently, $n_1 = n - \kappa - 1$. Thus G' is $(K_{n-\kappa-1} \cup K_1) + K_\kappa$. □

A pendant vertex is a vertex of degree one. Let $K_{n-k} \star S_{k+1}$ be obtained by joining k pendant vertices to one vertex of K_{n-k}. We study the $DD_{a,b}$ index for graphs with pendant vertices and show that $K_{n-k} \star S_{k+1}$ is the extremal graph.

Theorem 3.5. *Let G be any connected graph having order n and k pendant vertices, where $1 \leq k \leq n-3$. Then for $a \geq 1$ and $b \leq 0$, where $(a, b) \neq (1, 0)$,*

$$DD_{a,b}(G) \leq DD_{a,b}(K_{n-k} \star S_{k+1})$$

with equality only if G is $K_{n-k} \star S_{k+1}$.

Proof. Let G' be a graph with the largest $DD_{a,b}$ index with respect to order n and k pendant vertices. Let A be the set of pendant vertices of G'. By Lemma 2.2, there is an edge connecting each pair of vertices in $V(G') \setminus A$. So G' contains K_{n-k} as a subgraph. We prove that one vertex of that K_{n-k} is adjacent to all the k pendant vertices in G'.

Suppose to the contrary that K_{n-k} contains two vertices v and w, such that each of them is adjacent to a pendant vertex in G'. Let us denote the pendant neighbors of v by v_i where $i = 1, 2, \ldots, n_1$, and the pendant neighbors of w by w_j where $j = 1, 2, \ldots, n_2$. Clearly, n_1, n_2 are positive integers and $n_1 + n_2 \le k$. Without loss of generality, assume that $n_1 \ge n_2$. We compare the $DD_{a,b}$ indices of the graphs G' and G'' having the same vertex sets, where $E(G'') = \{vw_1, vw_2, \ldots, vw_{n_1}\} \cup E(G') \setminus \{ww_1, ww_2, \ldots, ww_{n_1}\}$.

We obtain $deg_{G'}(z) = deg_{G''}(z)$ and $S^b_{G'}(z) = S^b_{G''}(z)$ if z is not v, w, v_i, w_j, where $i = 1, 2, \ldots, n_1$ and $j = 1, 2, \ldots, n_2$. Let $s = n - k - 1$. Then $s \ge 2$. We have $deg_{G'}(v) = s + n_1$, $deg_{G'}(w) = s + n_2$, $deg_{G''}(v) = s + n_1 + n_2$ and $deg_{G''}(w) = s$. We obtain

$$\begin{aligned}
S^b_{G'}(v) &= (s + n_1) + 2^b(k - n_1),\\
S^b_{G'}(w) &= (s + n_2) + 2^b(k - n_2),\\
S^b_{G''}(v) &= (s + n_1 + n_2) + 2^b(k - n_1 - n_2),\\
S^b_{G''}(w) &= s + 2^b k,\\
S^b_{G'}(v_i) &= 1 + 2^b(s + n_1 - 1) + 3^b(k - n_1),\\
S^b_{G'}(w_j) &= 1 + 2^b(s + n_2 - 1) + 3^b(k - n_2),\\
S^b_{G''}(v_i) &= S^b_{G''}(w_j) = 1 + 2^b(s + n_1 + n_2 - 1) + 3^b(k - n_1 - n_2).
\end{aligned}$$

For $b \le 0$,

$$\begin{aligned}
S^b_{G'}(v_i) - S^b_{G''}(v_i) &= n_2(3^b - 2^b) \le 0,\\
S^b_{G'}(w_j) - S^b_{G''}(w_j) &= n_1(3^b - 2^b) \le 0.
\end{aligned}$$

For $b < 0$,

$$\begin{aligned}
S^b_{G''}(w) - S^b_{G'}(w) &= n_2(2^b - 1) < 0,\\
S^b_{G'}(w) - S^b_{G'}(v) &= (n_2 - n_1) + 2^b(n_1 - n_2) = (2^b - 1)(n_1 - n_2) \le 0,\\
S^b_{G'}(v) - S^b_{G''}(v) &= n_2(2^b - 1) < 0,
\end{aligned}$$

therefore

$$0 < S^b_{G''}(w) < S^b_{G'}(w) \le S^b_{G'}(v) < S^b_{G''}(v).$$

If $b = 0$, obviously $0 < S^b_{G''}(w) = S^b_{G'}(w) = S^b_{G'}(v) = S^b_{G''}(v)$. Note that

$$0 < s^a < (s + n_2)^a \le (s + n_1)^a < (s + n_1 + n_2)^a$$

for $a \ge 1$. Thus, for $a \ge 1$ and $b \le 0$, we obtain

$$\begin{aligned}
DD_{a,b}(G') - DD_{a,b}(G'') &= [deg_{G'}(v)]^a S^b_{G'}(v) - [deg_{G''}(v)]^a S^b_{G''}(v)\\
&\quad + [deg_{G'}(w)]^a S^b_{G'}(w) - [deg_{G''}(w)]^a S^b_{G''}(w)\\
&\quad + \sum_{i=1}^{n_1} ([deg_{G'}(v_i)]^a S^b_{G'}(v_i) - [deg_{G''}(v_i)]^a S^b_{G''}(v_i))\\
&\quad + \sum_{j=1}^{n_2} ([deg_{G'}(w_j)]^a S^b_{G'}(w_j) - [deg_{G''}(w_j)]^a S^b_{G''}(w_j))\\
&= (s + n_1)^a S^b_{G'}(v) - (s + n_1 + n_2)^a S^b_{G''}(v) + (s + n_2)^a S^b_{G'}(w)\\
&\quad - s^a S^b_{G''}(w) + n_1[S^b_{G'}(v_i) - S^b_{G''}(v_i)] + n_2[S^b_{G'}(w_j) - S^b_{G''}(w_j)]\\
&= (s + n_1)^a S^b_{G'}(v) - (s + n_1 + n_2)^a S^b_{G'}(v) + (s + n_2)^a S^b_{G'}(w)\\
&\quad - s^a S^b_{G'}(w) + (s + n_1 + n_2)^a [S^b_{G'}(v) - S^b_{G''}(v)]\\
&\quad + s^a [S^b_{G'}(w) - S^b_{G''}(w)] + 2n_1 n_2(3^b - 2^b)\\
&\le (s + n_1)^a S^b_{G'}(v) - (s + n_1 + n_2)^a S^b_{G'}(v)
\end{aligned}$$

$$\begin{aligned}&+ (s+n_2)^a S^b_{G'}(w) - s^a S^b_{G'}(w)\\ =\ & S^b_{G'}(v)[(s+n_1)^a - (s+n_1+n_2)^a] + S^b_{G'}(w)[(s+n_2)^a - s^a]\\ \le\ & S^b_{G'}(v)[(s+n_1)^a - (s+n_1+n_2)^a] + S^b_{G'}(v)[(s+n_2)^a - s^a]\\ \le\ & 0,\end{aligned}$$

since for $a = 1$, we have $(s+n_1)^a - (s+n_1+n_2)^a + (s+n_2)^a - s^a = 0$ and for $a > 1$, by Lemma 2.3,

$$(s+n_2)^a - s^a < (s+n_1+n_2)^a - (s+n_1)^a,$$

thus

$$(s+n_1)^a - (s+n_1+n_2)^a + (s+n_2)^a - s^a < 0.$$

So $DD_{a,b}(G') - DD_{a,b}(G'') < 0$ for $a > 1$ and $b \le 0$.

For $a \ge 1$ and $b < 0$, we have

$$S^b_{G'}(v) - S^b_{G''}(v) = S^b_{G''}(w) - S^b_{G'}(w) = n_2(2^b - 1) < 0,$$

thus

$$(s+n_1+n_2)^a[S^b_{G'}(v) - S^b_{G''}(v)] + s^a[S^b_{G'}(w) - S^b_{G''}(w)] < 0$$

and we again get $DD_{a,b}(G') - DD_{a,b}(G'') < 0$.

Therefore, $DD_{a,b}(G') < DD_{a,b}(G'')$ for $a \ge 1$ and $b \le 0$, where $(a,b) \ne (1,0)$. Thus G' is not a graph with the largest $DD_{a,b}$ index and we have a contradiction. Hence G' is $K_{n-k} \star S_{k+1}$. □

The problem studied in the previous theorem is trivial for $a = 1$ and $b = 0$. All graphs G with n vertices and m edges have the same $DD_{1,0}(G)$ index. We obtain

$$DD_{1,0}(G) = \sum_{v\in V(G)} \Big([deg_G(v)]^1 \sum_{w\in V(G)\setminus\{v\}} [d_G(v,w)]^0 \Big) = (n-1) \sum_{v\in V(G)} deg_G(v) = 2m(n-1).$$

So, by Lemma 2.2, each graph containing K_{n-k} and k pendant vertices is a graph with the largest $DD_{1,0}$ index with respect to order n and k pendant vertices.

Finally, we consider connected graphs without cycles called trees. In the following proof, we show that the diameter of the extremal tree T of given order is at most 2, which means that T is a star. Note that the distance between any two furthest vertices v and w is called the diameter of T and a shortest path between v and w is a diametral path.

Theorem 3.6. *Let T be any tree of order $n \ge 4$. Then for $a \ge 1$ and $b \le 0$, where $(a,b) \ne (1,0)$, we have*

$$DD_{a,b}(T) \le DD_{a,b}(S_n)$$

with equality only if T is S_n.

Proof. Let T' be a tree of order n with the largest $DD_{a,b}$ index. We prove that T' is S_n. If $n \le 3$, clearly T is S_n, so we study trees for $n \ge 4$.

Assume to the contrary that T' is not S_n. Thus the diameter of T' is $d \ge 3$. We denote a diametral path of T' by $u_0u_1u_2\dots u_d$, where $deg_{T'}(u_1) = n_1$ and $deg_{T'}(u_2) = n_2$. Clearly, $n_1, n_2 \ge 2$. So u_1 is adjacent to $n_1 - 1$ pendant vertices, say $v_1, v_2, \dots, v_{n_1-1}$ (one of them is u_0).

We compare the $DD_{a,b}$ indices of the trees T' and T'' having the same vertex sets, while the edge set $E(T'') = \{u_2v_1, u_2v_2, \dots, u_2v_{n_1-1}\} \cup E(T') \setminus \{u_1v_1, u_1v_2, \dots, u_1v_{n_1-1}\}$. We have $deg_{T''}(u_1) = 1$ and $deg_{T''}(u_2) = n_1 + n_2 - 1$. For $i = 1, 2, \dots, n_1 - 1$,

$$d_{T'}(u_1, v_i) = d_{T''}(u_2, v_i) = 1 \ \text{ and } \ d_{T''}(u_1, v_i) = d_{T'}(u_2, v_i) = 2,$$

thus for $b \leq 0$,

$$\begin{aligned} S^b_{T'}(u_1) - S^b_{T''}(u_1) &= (n_1 - 1)(1^b - 2^b) \geq 0, \\ S^b_{T'}(u_2) - S^b_{T''}(u_2) &= (n_1 - 1)(2^b - 1^b) \leq 0. \end{aligned}$$

Since $d_{T'}(u_1, z) = d_{T''}(u_2, z) + 1$ for each $z \in V(T') \setminus \{u_1, u_2, v_1, v_2, \ldots, v_{n_1-1}\}$, we get

$$[d_{T'}(u_1, z)]^b < [d_{T''}(u_2, z)]^b \quad \text{and} \quad S^b_{T'}(u_1) < S^b_{T''}(u_2)$$

for $b < 0$. Obviously,

$$[d_{T'}(u_1, z)]^b = [d_{T''}(u_2, z)]^b \quad \text{and} \quad S^b_{T'}(u_1) = S^b_{T''}(u_2)$$

for $b = 0$. For any z other than u_1, u_2 and v_i, where $i = 1, 2, \ldots, n_1 - 1$, we have $deg_{T'}(z) = deg_{T''}(z)$ and $d_{T'}(z, x) \geq d_{T''}(z, x)$, where $x \in V(T')$. For $b \leq 0$, we obtain $[d_{T'}(z, x)]^b \leq [d_{T''}(z, x)]^b$ and $S^b_{T'}(z) \leq S^b_{T''}(z)$, therefore

$$[deg_{T'}(z)]^a S^b_{T'}(z) \leq [deg_{T''}(z)]^a S^b_{T''}(z).$$

Similarly, $[deg_{T'}(v_i)]^a S^b_{T'}(v_i) \leq [deg_{T''}(v_i)]^a S^b_{T''}(v_i)$. Then, for $a \geq 1$ and $b \leq 0$,

$$\begin{aligned} DD_{a,b}(T') - DD_{a,b}(T'') &\leq [deg_{T'}(u_1)]^a S^b_{T'}(u_1) - [deg_{T''}(u_1)]^a S^b_{T''}(u_1) \\ &\quad + [deg_{T'}(u_2)]^a S^b_{T'}(u_2) - [deg_{T''}(u_2)]^a S^b_{T''}(u_2) \\ &= n_1^a S^b_{T'}(u_1) - 1^a S^b_{T''}(u_1) + n_2^a S^b_{T'}(u_2) - (n_1 + n_2 - 1)^a S^b_{T''}(u_2) \\ &= n_1^a S^b_{T'}(u_1) - S^b_{T'}(u_1) + n_2^a S^b_{T''}(u_2) - (n_1 + n_2 - 1)^a S^b_{T''}(u_2) \\ &\quad + [S^b_{T'}(u_1) - S^b_{T''}(u_1)] + n_2^a [S^b_{T'}(u_2) - S^b_{T''}(u_2)] \\ &\leq n_1^a S^b_{T'}(u_1) - S^b_{T'}(u_1) + n_2^a S^b_{T''}(u_2) - (n_1 + n_2 - 1)^a S^b_{T''}(u_2) \\ &= S^b_{T'}(u_1)[n_1^a - 1] + S^b_{T''}(u_2)[n_2^a - (n_1 + n_2 - 1)^a] \\ &\leq S^b_{T''}(u_2)[n_1^a - 1] + S^b_{T''}(u_2)[n_2^a - (n_1 + n_2 - 1)^a] \\ &\leq 0, \end{aligned}$$

since for $a = 1$, we have $n_1^a - 1 + n_2^a - (n_1 + n_2 - 1)^a = 0$ and for $a > 1$, by Lemma 2.3,

$$n_1^a - 1^a < (n_1 + n_2 - 1)^a - n_2^a,$$

thus

$$n_1^a - 1 + n_2^a - (n_1 + n_2 - 1)^a < 0.$$

So $DD_{a,b}(T') - DD_{a,b}(T'') < 0$ for $a > 1$ and $b \leq 0$.

For $a \geq 1$ and $b < 0$, we have $S^b_{T'}(u_1) < S^b_{T''}(u_2)$, thus

$$S^b_{T'}(u_1)[n_1^a - 1] < S^b_{T''}(u_2)[n_1^a - 1]$$

and we again get $DD_{a,b}(T') - DD_{a,b}(T'') < 0$.

Therefore, $DD_{a,b}(T') < DD_{a,b}(T'')$ for $a \geq 1$ and $b \leq 0$, where $(a, b) \neq (1, 0)$, which is a contradiction. Hence G' is S_n. □

Let us note that if $a = 1$ and $b = 0$, then all trees T of order n have the same $DD_{1,0}$ index, since

$$DD_{1,0}(T) = \sum_{v \in V(T)} \left([deg_T(v)]^1 \sum_{w \in V(T) \setminus \{v\}} [d_T(v, w)]^0 \right) = (n - 1) \sum_{v \in V(T)} deg_T(v) = 2(n - 1)^2.$$

4. Conclusion

We presented some bounds on the general degree distance for multipartite graphs and trees of given order, graphs of given order and chromatic number, graphs of given order and vertex connectivity, and graphs of given order and number of pendant vertices.

There is a huge space for further research, since one can study lower and upper bounds on the $DD_{a,b}$ index for general graphs or special classes of graphs for various invariants of graphs. Let us state the following problems.

Problem 4.1. *Find sharp upper and lower bounds on the $DD_{a,b}$ index for general graphs with respect to the order in combination with other graph invariants.*

Problem 4.2. *Find bounds on the $DD_{a,b}$ index for special classes of graphs such as bipartite graphs, trees and unicyclic graphs with respect to the order and one other graph invariant.*

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