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On Degree Distance of Hypergraphs

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Abstract

The degree distance of a connected hypergraph G is defined as

$$DD(G) = \sum_{u \in V(G)} d_u D_u,$$

where d_u is the degree of u, and D_u is the sum of distance between u and all other vertices of G. We determine the unique not necessarily uniform hypertree with the smallest (largest, respectively) degree distance among hypertrees with n vertices and m edges, where $1 \leq m \leq n-1$. We also determine the unique not necessarily uniform hypertrees with the first three smallest (largest, respectively) degree distances among hypertrees on $n \geq 5$ vertices. To obtain these results, we propose several local transformations on a hypergraph that decrease or increase the degree distance.

1 Introduction

A hypergraph G is an ordered pair $(V(G), E(G))$, where $V(G)$ is the vertex set and $E(G)$ is a family of subsets of $V(G)$, called the edge set of G. In this paper, $|e| \geq 2$ for $e \in E(G)$. If every edge of G has size k for some integer k, then G is k-uniform. A 2-uniform hypergraph is just a graph. The degree of a vertex v in G, denoted by $d_G(v)$ or d_v, is the number of edges of G containing v.

Hypergraph theory found applications in chemistry [14, 20, 21]. The study in [20] indicated that the hypergraph model gives a higher accuracy of molecular structure description: the higher the accuracy of the model, the greater the diversity of the behavior of its invariants.

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For $u, v \in V(G)$, a path from u to v in G is defined to be an alternating sequence of vertices and edges $(v_0, e_1, v_1, \ldots, v_{p-1}, e_p, v_p)$ with all v_i distinct and all e_i distinct such that for $i = 1, \ldots, p$, $\{v_{i-1}, v_i\} \subseteq e_i$, and if $j > i+1$, then $e_i \cap e_j = \emptyset$, where $v_0 = u$ and $v_p = v$. A cycle in G is defined to be an alternating sequence of vertices and edges $(v_0, e_1, v_1, \ldots, v_{p-1}, e_p, v_p)$ with $p \geq 2$, all v_i distinct except $v_0 = v_p$ and all e_i distinct such that for $i = 1, \ldots, p$, $\{v_{i-1}, v_i\} \subseteq e_i$, and if $|i-j| > 1$ with $\{i, j\} \neq \{1, p-1\}$, then $e_i \cap e_j = \emptyset$. The number of edges in a path or a cycle is its length. If there is a path from u to v for any $u, v \in V(G)$, then we say that G is connected. A hypertree is a connected hypergraph with no cycle. A k-uniform hypertree with m edges always has $1 + (k-1)m$ vertices.

Let G be a connected hypergraph. For $u, v \in V(G)$, the distance between u and v is the length of a shortest path from u and v in G, denoted by $d_G(u, v)$. In particular, $d_G(u, u) = 0$. The diameter of G is the maximum distance between all vertex pairs of G. The degree distance of G is defined as

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

That is

$$DD(G) = \sum_{u \in V(G)} d_G(u) D_G(u),$$

where, for $u \in V(G)$, $D_G(u)$ denotes the sum of distance between u and all other vertices of G, i.e., $D_G(u) = \sum_{v \in V(G)} d_G(u, v)$. For an ordinary connected graph, the degree distance was put forward by Dobrynin and Kochetova [6] and has been studied extensively, see, e.g., [1, 2, 6–8, 10, 16, 22, 25, 26]. Note that Schultz [24] introduced a graph invariant called molecular topological index, defined as the sum of the degree distance and the first Zagreb index (defined as the sum of the squares of the degrees), see, e.g. [12, 17, 18, 24].

The Wiener index of a connected hypergraph is defined as $W(G) = \sum_{\{u,v\} \subseteq V(G)} d_G(u, v)$. We mention that the Wiener index of a graph or hypergraph has been thoroughly studied, see, e.g. [3–5, 9, 11, 13, 15, 23, 27]. If G is a k-uniform hypertree with n vertices, where $2 \leq k \leq n$, Guo and Zhou [10] showed that $(k-1)DD(G) = 2kW(G) - n(n-1)$, extending the well known relation between the degree distance and the Wiener index of a tree, established in [12, 18]. Thus, the ordering of uniform hypertrees by degree distance coincides with the ordering by Wiener indices. But for general hypertrees that are not necessarily uniform, there is no such a relation between the degree distance and the Wiener index. For a connected hypergraph G, there is exactly one connected graph G^σ such that $V(D^\sigma) = V(G)$ and two vertices in G^σ are adjacent if and only if they belong to some edge of G. In this way, $W(G) = W(G^\sigma)$, but if one edge has size at least three, then $DD(G) \neq DD(G^\sigma)$.

In this paper, we study the degree distance of hypertrees that are not necessarily uniform. We determine the unique hypertree with the smallest (largest, respectively) degree distance among hypertrees with n vertices and m edges, where $1 \leq m \leq n-1$. We also determine the unique hypertrees with the first three smallest (largest, respectively) degree distances amon hypertrees on $n \geq 5$ vertices. To obtain these results, we propose several local transformations on a hypergraph that decrease or increase the degree distance.

2 Preliminaries

For a hypergraph G and $X \subseteq V(G)$ with $X \neq \emptyset$, let $G[X]$ be the subhypergraph induced by X, i.e., $G[X]$ has vertex set X and edge set $\{e \in E(G) : e \subseteq X\}$. For $v \in V(G)$, $G - v$ denotes the hypergraph with $V(G-v) = V(G) \setminus \{v\}$ and $E(G-v) = E(G) \setminus \{e : e \in E(G) \text{ and } v \in e\}$.

For a k-uniform hypertree G with $V(G) = \{v_1, \ldots, v_n\}$, if $E(G) = \{e_1, \ldots, e_m\}$ with $n - 1 = m(k-1)$, where $e_i = \{v_{(i-1)(k-1)+1}, \ldots, v_{(i-1)(k-1)+k}\}$ for $i = 1, \ldots, m$, then we call G a k-uniform loose path, denoted by $P_{n,k}$. Denote $P_n = P_{n,2}$.

For a k-uniform hypertree G on n vertices, if there is a disjoint partition of the vertex set $V(G) = \{v_0\} \cup V_1 \cup \ldots \cup V_m$ such that $|V_1| = \cdots = |V_m| = k-1$, and $E(G) = \{\{v_0\} \cup V_i : 1 \leq i \leq m\}$, then we call G a k-uniform hyperstar (with center v_0), denoted by $S_{n,k}$. In particular, $S_{k,k}$ is a hypergraph with a single edge.

A path $(v_0, e_1, v_1, \ldots, v_{s-1}, e_s, v_s)$ in a k-uniform hypergraph G is called a pendant path at v_0, if $d_G(v_0) \geq 2$, $d_G(v_i) = 2$ for $1 \leq i \leq s-1$, $d_G(v) = 1$ for $v \in e_i \setminus \{v_{i-1}, v_i\}$ with $1 \leq i \leq s$, and $d_G(v_s) = 1$. An edge $e = \{w_1, \ldots, w_k\}$ in G is called a pendant edge at w_1 if $d_G(w_1) \geq 2$, and $d_G(w_i) = 1$ for $2 \leq i \leq k$.

If P is a pendant path of length s at u in a hypergraph G, we say G is obtained from H by attaching a pendant path of length s at u, where $H = G[V(G) \setminus (V(P) \setminus \{u\})]$. If P is a pendant path of length 1 at u in G, then we also say that G is obtained from H by attaching a pendant edge at u.

Let r be a positive integer and G a hypergraph with $u, v_1, \ldots, v_r \in V(G)$ and $e_1, \ldots, e_r$

$\in E(G)$ such that $u \notin e_i$, $v_i \in e_i$, and $e_i' \notin E(G)$ for $1 \leq i \leq r$, where $e_i' = (e_i \setminus \{v_i\}) \cup \{u\}$ and $v_1, \ldots, v_r$ are not necessarily pairwise distinct. Let G' be the hypergraph with $V(G') = V(G)$ and $E(G') = (E(G) \setminus \{e_1, \ldots, e_r\}) \cup \{e_1', \ldots, e_r'\}$. Then we say that G' is obtained from G by moving edges $e_1, \ldots, e_r$ from $v_1, \ldots, v_r$ to u.

Let G be a hypergraph with $e_1, e_2 \in E(G)$ and $u_1, \ldots, u_s \in V(G)$ such that $u_1, \ldots, u_s \notin e_1$ and $u_1, \ldots, u_s \in e_2$, where $|e_2| - s \geq 2$. Let $e_1' = e_1 \cup \{u_1, \ldots, u_s\}$ and $e_2' = e_2 \setminus \{u_1, \ldots, u_s\}$. Suppose that $e_1', e_2' \notin E(G)$. Let G' be the hypergraph with $V(G') = V(G)$ and $E(G') = (E(G) \setminus \{e_1, e_2\}) \cup \{e_1', e_2'\}$. Then we say that G' is obtained from G by moving vertices $u_1, \ldots, u_s$ from e_2 to e_1.

For $k \geq 3$, let $e = \{w_1, \ldots, w_k\}$ be an edge of a hypergraph G. Let $e_1 = \{w_1, w_2\}$ and $e_2 = e \setminus \{w_2\}$. Suppose that $e_1, e_2 \notin E(G)$. Let G' be the hypergraph with $V(G') = V(G)$ and $E(G') = (E(G) \setminus \{e\}) \cup \{e_1, e_2\}$. Then we say that G' is obtained from G by moving vertex w_2 from e and adding an edge $\{w_1, w_2\}$.

3 Local transformations and degree distance

In this section, we propose some local transformations on a hypergraph that decrease or increase the degree distance. Two different vertices are adjacent in a hypergraph if there is an edge containing both of them. For a vertex u of a hypergraph G, let $N_G(u)$ be the set of vertices adjacent to u in G.

Theorem 1. *Let G be a hypergraph with connected induced subhypergraphs G_0, H_1 and H_2 such that there are two adjacent vertices w_1 and w_2 in G_0 with $N_{G_0}(w_1) \setminus \{w_2\} = N_{G_0}(w_2) \setminus \{w_1\}$, $d_{G_0}(w_1) = d_{G_0}(w_2)$ and $V(H_i) \cap V(G_0) = \{w_i\}$ for $i = 1, 2$, $V(H_1) \cap V(H_2) = \varnothing$ and $E(G) = E(G_0) \cup E(H_1) \cup E(H_2)$. Suppose that $|V(H_i)| \geq 2$ for $i = 1, 2$. Let G' be the hypergraph obtained from G by moving all edges containing w_2 except edges in $E(G_0)$ from w_2 to w_1. Then $DD(G') < DD(G)$.*

Proof. Let $h_1 = |V(H_1)|$ and $h_2 = |V(H_2)|$. As we pass from G to G', the distance between a vertex of $V(H_2) \setminus \{w_2\}$ and a vertex of $V(H_1)$ is decreased by 1, the distance between a vertex of $V(H_2) \setminus \{w_2\}$ and w_2 is increased by 1, and the distance between any other vertex pair remains unchanged. Note also that for any $x \in V(G_0) \setminus \{w_1, w_2\}$, we have $d_{G_0}(x, w_1) = d_{G_0}(x, w_2)$ as $N_{G_0}(w_1) \setminus \{w_2\} = N_{G_0}(w_2) \setminus \{w_1\}$. Thus

$$D_{G'}(x) - D_G(x) = \begin{cases} -(h_2 - 1) & \text{if } x \in V(H_1), \\ -(h_1 - 1) & \text{if } x \in V(H_2) \setminus \{w_2\}, \\ h_2 - 1 & \text{if } x = w_2, \\ 0 & \text{if } x \in V(G_0) \setminus \{w_1, w_2\}. \end{cases}$$

Note that $d_{G'}(x) = d_G(x)$ for $x \in V(G) \setminus \{w_1, w_2\}$. Let $a = d_G(w_1)$, $b = d_G(w_2)$ and $t = d_{H_2}(w_2)$. Then $d_{G'}(w_1) = a + t$ and $d_{G'}(w_2) = b - t$. Therefore

$$\begin{aligned} & DD(G') - DD(G) \\ = & \sum_{u \in V(H_1) \setminus \{w_1\}} d_G(u)(D_{G'}(u) - D_G(u)) + \sum_{v \in V(H_2) \setminus \{w_2\}} d_G(v)(D_{G'}(v) - D_G(v)) \\ & +(a+t)D_{G'}(w_1) - aD_G(w_1) + (b-t)D_{G'}(w_2) - bD_G(w_2) \\ = & -(h_2 - 1) \sum_{u \in V(H_1) \setminus \{w_1\}} d_G(u) - (h_1 - 1) \sum_{v \in V(H_2) \setminus \{w_2\}} d_G(v) \\ & +(a+t)(D_G(w_1) - h_2 + 1) - aD_G(w_1) \\ & +(b-t)(D_G(w_2) + h_2 - 1) - bD_G(w_2) \\ < & (a+t)(D_G(w_1) - h_2 + 1) - aD_G(w_1) \\ & +(b-t)(D_G(w_2) + h_2 - 1) - bD_G(w_2) \\ = & -ah_2 + a + tD_G(w_1) - th_2 + t + bh_2 - b - tD_G(w_2) - th_2 + t \\ = & (b-a)(h_2 - 1) + t(D_G(w_1) - D_G(w_2)) - 2th_2 + 2t. \end{aligned}$$

As

$$\begin{aligned} D_G(w_1) - D_G(w_2) &= D_{G_0}(w_1) + D_{H_1}(w_1) + D_{H_2}(w_2) + h_2 - 1 \\ &\quad - (D_{G_0}(w_2) + D_{H_2}(w_2) + D_{H_1}(w_1) + h_1 - 1) \\ &= h_2 - h_1, \end{aligned}$$

and $b - a = d_G(w_2) - d_G(w_1) = d_{H_2}(w_2) - d_{H_1}(w_1) = t - d_{H_1}(w_1) \le t - 1$, we have

$$\begin{aligned} DD(G') - DD(G) &< (b-a)(h_2 - 1) + t(h_2 - h_1) - 2th_2 + 2t \\ &= (b - a - t)(h_2 - 1) - t(h_1 - 1) \\ &< 0, \end{aligned}$$

implying that $DD(G') < DD(G)$. ■

Theorem 2. *For $k-2 \geq r \geq 1$, let G be a connected hypergraph with two pendant edges $e_1 = \{u, w_1, \ldots, w_k\}$ and $e_2 = \{u, v_1, \ldots, v_r\}$. Let G' be the hypergraph obtained from G by moving vertex w_1 from e_1 to e_2. Then $DD(G') > DD(G)$.*

Proof. As we pass from G to G', the distance between w_1 and a vertex of $e_1 \setminus \{u, w_1\}$ is increased by 1, the distance between w_1 and a vertex of $e_2 \setminus \{u\}$ is decreased by 1, and the distance between any other vertex pair remains unchanged. Thus

$$\begin{aligned} D_{G'}(w_1) - D_G(w_1) &= k - r - 1, \\ D_{G'}(w_i) - D_G(w_i) &= 1 \text{ if } 2 \leq i \leq k, \\ D_{G'}(v_j) - D_G(v_j) &= -1 \text{ if } 1 \leq j \leq r, \\ D_{G'}(x) - D_G(x) &= 0 \text{ if } x \in V(G) \setminus ((e_1 \cup e_2) \setminus \{u\}). \end{aligned}$$

Therefore

$$\begin{aligned} DD(G') - DD(G) &= \sum_{i=1}^{k}(D_{G'}(w_i) - D_G(w_i)) + \sum_{j=1}^{r}(D_{G'}(v_i) - D_G(v_i)) \\ &= k - r - 1 + (k-1) \cdot 1 + r \cdot (-1) \\ &= 2(k - r - 1) > 0, \end{aligned}$$

i.e., $DD(G') > DD(G)$. ■

Theorem 3. *For $k \geq 3$, let $e = \{w_1, w_2, \ldots, w_k\}$ be an edge of a connected hypergraph G. Let G' be the hypergraph obtained from G by moving vertex w_2 from e and attaching an edge $\{w_1, w_2\}$ to w_1. Suppose that w_2 and some vertex in $e \setminus \{w_1, w_2\}$ are not adjacent in G'. Then $DD(G') > DD(G)$.*

Proof. We may assume that w_2 and w_3 are not adjacent in G'. As we pass from G to G', the distance between w_2 and w_3 is increased by 1, and the distance between any other vertex pair is increased or remains unchanged. That is, $D_{G'}(x) \geq D_G(x)$ for $x \in V(G) \setminus \{w_1, w_2\}$, and $D_{G'}(w_1) = D_G(w_1)$, $D_{G'}(w_2) \geq D_G(w_2) + 1$. Note also that $d_{G'}(x) = d_G(x)$ for $x \in V(G) \setminus \{w_1\}$. Thus

$$\begin{aligned} DD(G') - DD(G) &\geq (d_G(w_1) + 1)D_{G'}(w_1) - d_G(w_1)D_G(w_1) \\ &\quad + d_{G'}(w_2)D_{G'}(w_2) - d_G(w_2)D_G(w_2) \\ &\geq D_G(w_1) + d_G(w_2) > 0, \end{aligned}$$

i.e., $DD(G') > DD(G)$. ■

Theorem 4. *Let t be an integer with $t \geq 3$ and G a hypergraph consisting of t connected subhypergraphs $G_1, \ldots, G_t$ such that $|V(G_i)| \geq 2$ for $i = 1, \ldots, t$ and $V(G_i) \cap V(G_j) = \{u\}$ for $1 \leq i < j \leq t$. Let $e_1 = \{u, v_1, \ldots\} \in E(G_1)$, $e_2 = \{u, v_2, \ldots\} \in E(G_2)$. Let G' (G'', respectively) be the hypergraph obtained from G by moving all the edges containing u in G_i for all $i = 3, \ldots, t$ from u to v_1 (v_2, respectively). Then $DD(G) < \max\{DD(G'), DD(G'')\}$.*

Proof. Let $g_i = |V(G_i)|$ for $i = 1, \ldots, t$. As we pass from G to G', the distance between a vertex of $\bigcup_{i=3}^{t} V(G_i) \setminus \{u\}$ and a vertex of $V(G_1) \setminus \{u\}$ is decreased by at most 1, the distance between a vertex of $\bigcup_{i=3}^{t} V(G_i) \setminus \{u\}$ and a vertex of $V(G_2)$ is increased by 1, and the distance between any other vertex pair remains unchanged. Thus

$$D_{G'}(x) - D_G(x) \geq \begin{cases} -\sum_{i=3}^{t}(g_i - 1) & \text{if } x \in V(G_1) \setminus \{u\}, \\ \sum_{i=3}^{t}(g_i - 1) & \text{if } x \in V(G_2), \\ g_2 - (g_1 - 1) & \text{if } x \in \bigcup_{i=3}^{t} V(G_i) \setminus \{u\}. \end{cases}$$

Let $a = d_G(u)$ and $\ell = \sum_{i=3}^{t} d_{G_i}(u)$. Then $d_{G'}(u) = a - \ell$ and $d_{G'}(v_1) = d_G(v_1) + \ell$. Note that $d_{G'}(x) = d_G(x)$ for $x \in V(G) \setminus \{u, v_1\}$. Let $\delta_i = \sum_{x \in V(G_i) \setminus \{u\}} d_G(x)$ for $i = 1, \ldots, t$. Therefore

$$\begin{aligned} & DD(G') - DD(G) \\ = & \sum_{x \in V(G_1) \setminus \{u, v_1\}} d_G(x)(D_{G'}(x) - D_G(x)) + \sum_{x \in V(G_2) \setminus \{u\}} d_G(x)(D_{G'}(x) - D_G(x)) \\ & + \sum_{x \in \bigcup_{i=3}^{t}(V(G_i) \setminus \{u\})} d_G(x)(D_{G'}(x) - D_G(x)) + (a - \ell)D_{G'}(u) - aD_G(u) \\ & + (d_G(v_1) + \ell)D_{G'}(v_1) - d_G(v_1)D_G(v_1) \\ \geq & -\sum_{x \in V(G_1) \setminus \{u, v_1\}} d_G(x) \sum_{i=3}^{t}(g_i - 1) + \sum_{x \in V(G_2) \setminus \{u\}} d_G(x) \sum_{i=3}^{t}(g_i - 1) \\ & + \sum_{x \in \bigcup_{i=3}^{t}(V(G_i) \setminus \{u\})} d_G(x)(g_2 - (g_1 - 1)) + a\sum_{i=3}^{t}(g_i - 1) - \ell D_{G'}(u) \\ & - d_G(v_1)\sum_{i=3}^{t}(g_i - 1) + \ell D_{G'}(v_1) = -(\delta_1 - d_G(v_1))\sum_{i=3}^{t}(g_i - 1) + \delta_2 \sum_{i=3}^{t}(g_i - 1) \end{aligned}$$

$$
\begin{aligned}
&+\left(\sum_{i=3}^{t}\delta_i\right)(1+g_2-g_1)+a\sum_{i=3}^{t}(g_i-1)\\
&-d_G(v_1)\sum_{i=3}^{t}(g_i-1)+\ell(D_{G'}(v_1)-D_{G'}(u))\\
=\;&(-\delta_1+\delta_2+a)\sum_{i=3}^{t}(g_i-1)+\left(\sum_{i=3}^{t}\delta_i\right)(1+g_2-g_1)\\
&+\ell(D_{G'}(v_1)-D_{G'}(u)).
\end{aligned}
$$

Note that

$$
\begin{aligned}
D_{G'}(v_1)-D_{G'}(u) &= \sum_{w\in V(G)\setminus V(G_2)}(d_{G'}(v_1,w)-d_{G'}(u,w))\\
&\quad+\sum_{w\in V(G_2)}(d_{G'}(v_1,w)-d_{G'}(u,w))\\
&\geq \sum_{w\in V(G)\setminus V(G_2)}(-1)+\sum_{w\in V(G_2)}1\\
&= -(g_1-1)-\sum_{i=3}^{t}(g_i-1)+g_2\\
&= -\sum_{i=3}^{t}(g_i-1)+1+g_2-g_1.
\end{aligned}
$$

Therefore

$$
\begin{aligned}
DD(G')-DD(G) &\geq (-\delta_1+\delta_2+a-\ell)\sum_{i=3}^{t}(g_i-1)\\
&\quad+\left(\ell+\sum_{i=3}^{t}\delta_i\right)(1+g_2-g_1).
\end{aligned}
$$

Similarly,

$$
\begin{aligned}
DD(G'')-DD(G) &\geq (-\delta_2+\delta_1+a-\ell)\sum_{i=3}^{t}(g_i-1)\\
&\quad+\left(\ell+\sum_{i=3}^{t}\delta_i\right)(1+g_1-g_2).
\end{aligned}
$$

Thus

$$
\begin{aligned}
DD(G')-DD(G)+DD(G'')-DD(G) &\geq 2(a-\ell)\sum_{i=3}^{t}(g_i-1)\\
&\quad+2\left(\ell+\sum_{i=3}^{t}\delta_i\right)\\
&> 0,
\end{aligned}
$$

implying that $DD(G)<\max\{DD(G'),DD(G'')\}$. ■

Theorem 5. *Let t be an integer with $t \geq 3$ and G a hypergraph with an edge $e = \{w_1, \dots, w_t\}$ such that $G - e$ consists of vertex-disjoint connected subhypergraphs $H_1, \dots, H_t$, each containing exactly one vertex of e. Let $e \cap V(H_i) = \{w_i\}$ for $i = 1, \dots, t$. Let $w_1 \in e_1 \in E(H_1)$, $w_2 \in e_2 \in E(H_2)$. Let G' (G'', respectively) be the hypergraph obtained from G by moving $w_3, \dots, w_t$ from e to e_1 (e_2, respectively). Then $DD(G) < \max\{DD(G'), DD(G'')\}$.*

Proof. Let $h_i = |V(H_i)|$ for $i = 1, \dots, t$. As we pass from G to G', the distance between a vertex of $\bigcup_{i=3}^{t} V(H_i)$ and a vertex of $V(H_1)$ is decreased by at most 1, the distance between a vertex of $\bigcup_{i=3}^{t} V(H_i)$ and a vertex of $V(H_2)$ is increased by 1, and the distance between any other vertex pair remains unchanged. Then $D_{G'}(x) - D_G(x) \geq -\sum_{i=3}^{t} h_i$ for $x \in V(H_1)$, $D_{G'}(x) - D_G(x) = \sum_{i=3}^{t} h_i$ for $x \in V(H_2)$, and $D_{G'}(x) - D_G(x) \geq h_2 - (h_1 - 1) = 1 + h_2 - h_1$ for $x \in \bigcup_{i=3}^{t} V(H_i)$. Note that $d_{G'}(x) = d_G(x)$ for $x \in V(G)$. Let $\delta_i = \sum_{x \in V(H_i)} d_G(x)$ for $i = 1, \dots, t$. Thus

$$
\begin{aligned}
DD(G') - DD(G) &= \sum_{x \in V(H_1)} d_G(x)(D_{G'}(x) - D_G(x)) \\
&\quad + \sum_{x \in V(H_2)} d_G(x)(D_{G'}(x) - D_G(x)) \\
&\quad + \sum_{x \in \bigcup_{i=3}^{t} V(H_i)} d_G(x)(D_{G'}(x) - D_G(x)) \\
&\geq \delta_1(-\sum_{i=3}^{t} h_i) + \delta_2 \sum_{i=3}^{t} h_i + \left(\sum_{i=3}^{t} \delta_i\right)(1 + h_2 - h_1) \\
&= (\delta_2 - \delta_1) \sum_{i=3}^{t} h_i + \left(\sum_{i=3}^{t} \delta_i\right)(1 + h_2 - h_1).
\end{aligned}
$$

Similarly,

$$DD(G'') - DD(G) \geq (\delta_1 - \delta_2) \sum_{i=3}^{t} h_i + \left(\sum_{i=3}^{t} \delta_i\right)(1 + h_1 - h_2).$$

Thus

$$DD(G') - DD(G) + DD(G'') - DD(G) \geq 2 \sum_{i=3}^{t} \delta_i > 0,$$

implying that $DD(G) < \max\{DD(G'), DD(G'')\}$. ■

4 Hypertrees with small degree distances

For $1 \le m \le n-1$, let S_n^m be the hyperstar on n vertices with $m-1$ pendant edges of size 2 and one pendant edge of size $n-m+1$ (at its center).

Theorem 6. *Let T be a hypertree on n vertices with m edges, where $1 \le m \le n-1$. Then*

$$DD(T) \ge n^2 + (3m-4)n - (m+3)(m-1)$$

with equality if and only if $T \cong S_n^m$.

Proof. By direct calculation, we have $DD(S_n^m) = m(n-1) + 1 \cdot (1 + 2(n-2)) \cdot (m-1) + 1 \cdot (n-m+2(m-1)) \cdot (n-m) = n^2 + (3m-4)n - (m+3)(m-1)$.

If $m = 1$, then it is evident that $T \cong S_n^1$ with $DD(T) = n(n-1) = n^2 - n$, and so the result follows.

Suppose that $m \ge 2$. Let T be a hypertree on n vertices with m edges that minimizes the degree distance.

Suppose that there is an edge $e \in E(T)$ containing two vertices, say w_1 and w_2, of degree at least two. Let T' be the hypertree obtained from T by moving all edges containing w_2 except e from w_2 to w_1. By Theorem 1, $DD(T) > DD(T')$, a contradiction. Thus all the m edges of T are pendant edges at a common vertex, i.e., T is a hyperstar.

Let $a_1, \ldots, a_m$ be the sizes of the m edges of T. Obviously, $\sum_{i=1}^{m} a_i = n+m-1$. Assume that $a_1 \ge \cdots \ge a_m \ge 2$. Suppose that $a_2 \ge 3$. Let e_1 and e_2 be two edges of T with $|e_1| = a_1$ and $|e_2| = a_2$. Let T'' be the hypertree obtained from T by moving a vertex of degree one in e_2 from e_2 to e_1. By Theorem 2, $DD(T) > DD(T'')$, a contradiction. Thus $a_2 = 2$ and $a_1 = n-m+1$. That is, $T \cong S_n^m$. ■

Lemma 1. *If $1 \le m < n-1$, then $DD(S_n^m) < DD(S_n^{m+1})$.*

Proof. Let $T = S_n^m$ with center u and edge e of size $n-m+1$. Let T' be the hypertree obtained from T by moving one vertex, say w, in $e \setminus \{u\}$ from e and adding an edge $\{u, w\}$. Evidently, $T \cong S_n^{m+1}$. By Theorem 3, $DD(S_n^m) < DD(S_n^{m+1})$. ■

Corollary 1. *Let T be a hypertree on n vertices with maximum degree s or with s pendant edges, where $1 \le s \le n-1$. Then $DD(T) \ge DD(S_n^s)$ with equality if and only if $T \cong S_n^s$.*

Proof. Since $|E(T)| \ge s$, we have by Theorem 6 and Lemma 1 that $DD(T) \ge DD(S_n^{|E(T)|})$ $\ge DD(S_n^s)$ with equalities if and only if $T \cong S_n^{|E(T)|}$ and $|E(T)| = s$, i.e., $T \cong S_n^s$. ■

For $n \geq 5$, let T_n^2 be the hyperstar on n vertices with one pendant edge of size 3 and one pendant edge of size $n-2$.

Theorem 7. *Among hypertrees on n vertices,*

- $n^2 - n$ *for* $n \geq 1$ *is the smallest degree distance, achieved uniquely by* S_n^1*;*
- $n^2 + 2n - 5$ *for* $n \geq 3$ *is the second smallest degree distance, achieved uniquely by* S_n^2*;*
- 24 *for* $n = 4$ *and* $n^2 + 4n - 13$ *for* $n \geq 5$ *are the third smallest degree distances, achieved uniquely by* S_4^3 *and* T_n^2*, respectively.*

Proof. Let T be a hypertree on n vertices that is not isomorphic to S_n^1, S_n^2. Let m be the number of edges of T. As $T \not\cong S_n^1$, we have $m \geq 2$. Suppose that $m \geq 3$. Then $n \geq 4$. If $n = 4$, then, as $T \not\cong S_n^1, S_n^2$, we have $T \cong P_{4,2}, S_4^3$, and by Theorem 1, $DD(P_{4,2}) > DD(S_4^3)$. If $n \geq 5$, then by Theorem 6, Lemma 1 and Theorem 2, we have $DD(T) \geq DD(S_n^m) \geq DD(S_n^3) > DD(T_n^2)$. If $m = 2$, then, as $T \not\cong S_n^2$, we have by by Theorem 2 that $DD(T) \geq DD(T_n^2)$ with equality if and only if $T \cong T_n^2$. By direct calculation,

$$\begin{aligned} DD(T_n^2) &= 2(2 + 2(n-3)) + (n-3)(4 + n - 3) + 2(n-1) \\ &= n^2 + 4n - 13. \end{aligned}$$

Thus, we have either $n = 4$ and $DD(T) \geq 24$ with equality if and only if $T \cong S_4^3$ or $n \geq 5$ and $DD(T) \geq n^2 + 4n - 13$ with equality if and only if $T \cong T_n^2$.

Now the result follows by noting that $DD(S_n^1) = n^2 - n$ and $DD(S_n^2) = n^2 + 2n - 5$. ■

5 Hypertrees with large degree distances

For $2 \leq m \leq n-1$ and $2 \leq k \leq r \leq n-1$, let $P_n^m(k,r) = (v_0, e_1, v_1, e_2, \ldots, e_m, v_m)$ be a path on n vertices with m edges such that $|e_1| = k$, $|e_m| = r$, $|e_i| = 2$ for $i = 2, \ldots, m-1$, and $k + r = n - m + 3$. If $r - k = 0, 1$, then we write P_n^m instead of $P_n^m(k,r)$. Obviously, $P_n^{n-1} \cong P_{n,2}$. Note that $P_n^m(k,r)$ is obtainable from the path $P_{m-1,2}$ by attaching a pendant edge of size k to one terminal vertex and a pendant edge of size r to the other terminal vertex.

Let $P_n^1 = S_n^1$.

Lemma 2. *For $2 \leq k \leq r$, $m \geq 2$ and $n = k + r + m - 3$,*

$$\begin{aligned} DD(P_n^m(k,r)) &= \frac{1}{6}m(m-1)(9n-5m+1) + 2m(k-1)(r-1) \\ &\quad +(k-1)(k-2)+(r-1)(r-2). \end{aligned}$$

Proof. By direct calculation, we have

$$\begin{aligned}
& DD(P_n^m(k,r)) \\
= \; & (k-1)\left(k-2+\sum_{i=1}^{m-1} i + (r-1)m\right) \\
& +(r-1)\left(r-2+\sum_{i=1}^{m-1} i + (k-1)m\right) \\
& +2\sum_{j=1}^{m-1}\left(\sum_{i=0}^{j-1} i + (k-1)j + \sum_{i=0}^{m-1-j} i + (r-1)(m-j)\right) \\
= \; & (k-1)\left(k-2+\frac{1}{2}m(m-1)+(r-1)m\right) \\
& +(r-1)\left(r-2+\frac{1}{2}m(m-1)+(k-1)m\right) \\
& +\sum_{j=1}^{m-1}\left(j(j-1)+2(k-1)j+(m-j)(m+2r-3-j)\right) \\
= \; & (k-1)(k-2)+(r-1)(r-2)+\frac{1}{2}m(m-1)(k+r-2) \\
& +2m(k-1)(r-1) \\
& +\sum_{j=1}^{m-1}\left(2j^2-2(m-k+r)j+m(m+2r-3)\right) \\
= \; & (k-1)(k-2)+(r-1)(r-2)+\frac{1}{2}m(m-1)(k+r-2) \\
& +2m(k-1)(r-1) \\
& +\frac{1}{3}m(m-1)(2m+3k+3r-10) \\
= \; & \frac{1}{6}m(m-1)(9n-5m+1)+2m(k-1)(r-1) \\
& +(k-1)(k-2)+(r-1)(r-2),
\end{aligned}$$

as desired. ■

Lemma 3. *For $2 \leq k \leq r-2$, $m \geq 2$ and $n = k + r + m - 3$,*

$$DD(P_n^m(k,r)) < DD(P_n^m(k+1,r-1)).$$

Proof. By Lemma 2, we have

$$\begin{aligned} & DD(P_n^m(k+1,r-1)) - DD(P_n^m(k,r)) \\ = & \; 2m\left(k(r-2)-(k-1)(r-1)\right)+k(k-1) \\ & -(k-1)(k-2)+(r-2)(r-3)-(r-1)(r-2) \\ = & \; 2m(r-k-1)+(2k-2)-2r+4 \\ = & \; 2(m-1)(r-k-1) \\ > & \; 0. \end{aligned}$$

So the result follows. ■

Lemma 4. *For $n > m \geq 2$,*

$$DD(P_n^m) = \begin{cases} \frac{1}{6}\left(3(m+1)n^2+3m(m-3)n-(2m-3)(m^2-1)\right) & \text{if } n-m \text{ is odd,} \\ \frac{1}{6}\left(3(m+1)n^2+3m(m-3)n-(2m-1)(m^2-m)\right) & \text{if } n-m \text{ is even.} \end{cases}$$

Proof. Recall that $P_n^m = P_n^m(k,r)$, where $k+r = n-m+3$ and $r-k = 0,1$.

If $n-m$ is odd, then $k = r = \frac{1}{2}(n-m+3)$, and we have by Lemma 2 that

$$\begin{aligned} DD(P_n^m) = & \; \frac{1}{6}m(m-1)(9n-5m+1)+2m\left(\frac{n-m+1}{2}\right)^2 \\ & +2\cdot\frac{n-m+1}{2}\cdot\frac{n-m-1}{2} \\ = & \; \frac{1}{6}m(m-1)(9n+1)-\frac{5}{6}m^2(m-1) \\ & +\frac{m}{2}(n^2+m^2+1-2mn+2n-2m)+\frac{1}{2}(n^2-2mn+m^2-1) \\ = & \; \frac{1}{6}\left(3(m+1)n^2+3m(m-3)n-(2m-3)(m^2-1)\right). \end{aligned}$$

If $n-m$ is even, then $k = \frac{1}{2}(n-m+2)$, $r = \frac{1}{2}(n-m+4)$, and we have by Lemma 2 that

$$\begin{aligned} DD(P_n^m) = & \; \frac{1}{6}m(m-1)(9n-5m+1)+2m\cdot\frac{n-m}{2}\cdot\frac{n-m+2}{2} \\ & +\frac{n-m}{2}\cdot\frac{n-m-2}{2}+\frac{n-m}{2}\cdot\frac{n-m+2}{2} \\ = & \; \frac{1}{6}m(m-1)(9n+1)-\frac{5}{6}m^2(m-1) \\ & +\frac{m}{2}(n^2-2mn+m^2+2n-2m)+\frac{1}{2}(n^2-2mn+m^2) \\ = & \; \frac{1}{6}\left(3(m+1)n^2+3m(m-3)n-(2m-1)(m^2-m)\right). \end{aligned}$$

This completes the proof. ■

Theorem 8. *Let T be a hypertree on n vertices with m edges, where $1 \le m \le n-1$. Then*

$$DD(T) \le \begin{cases} \frac{1}{6}\left(3(m+1)n^2 + 3m(m-3)n - (2m-3)(m^2-1)\right) & \text{if } n-m \text{ is odd} \\ \frac{1}{6}\left(3(m+1)n^2 + 3m(m-3)n - (2m-1)(m^2-m)\right) & \text{if } n-m \text{ is even} \end{cases}$$

with equality if and only if $T \cong P_n^m$.

Proof. It is trivial if $m = 1$.

Suppose that $m \ge 2$. Let T be a hypertree on n vertices with m edges maximizing the degree distance.

Suppose that there is a vertex u in T of degree at least three. Let $d_T(u) = t \ge 3$. Then T consists of t subhypertrees $T_1, \dots, T_t$ such that $|V(T_i)| \ge 2$ for $1 \le i \le t$ and $T_1, \dots, T_t$ have exactly one vertex u in common. Let $e_1 = (u, v_1, \dots) \in E(T_1)$, $e_2 = (u, v_2, \dots) \in E(T_2)$ and let T' (T'', respectively) be the hypertree obtained from T by moving all the edges containing u in each of $T_3, \dots, T_t$ from u to v_1 (v_2, respectively). Obviously, T' and T'' also have m edges. By Theorem 4, $DD(T) < \max\{DD(T'), DD(T'')\}$, a contradiction. Thus the maximum degree of T is two.

Suppose that there is an edge in T of size at least three, whose deletion yields at least two nontrivial components. Let $e = \{w_1, \dots, w_k\}$ be such one edge, where $k \ge 3$. For $i = 1, \dots, k$, let T_i be the component in $T - e$ containing w_i. Let $w_1 \in e_1 \in E(T_1)$, $w_2 \in e_2 \in E(T_2)$ and T^* (T^{**}, respectively) be the hypertree obtained from T by moving $w_3, \dots, w_k$ from e to e_1(e_2, respectively). Obviously, T^* and T^{**} also have m edges. By Theorem 5, $DD(T) < \max\{DD(T^*), DD(T^{**})\}$, a contradiction. Thus, the deletion of any edge of size at least three yields exactly one nontrivial component. That is any edge of size at least three in T is a pendant edge. As the maximum degree of T is two, we conclude that $T \cong P_n^m(k, r)$, where $2 \le k \le r$. Now by Lemma 3, $T \cong P_n^m$. Now the result follows from Lemma 4. ■

Lemma 5. *If $1 \le m < n-1$, then $DD(P_n^m) < DD(P_n^{m+1})$.*

Proof. Let $P_n^m = (v_0, e_1, v_1, e_2, \dots, v_{m-1}, e_m, v_m)$ such that $|e_1| + |e_m| = n - m + 3$ and $|e_m| - |e_1| = 0, 1$.

Since $m < n-1$, we have $|e_m| \ge 3$. Let $u \in e_m \setminus \{v_{m-1}, v_m\}$, $e = \{v_{m-1}, u\}$ and $e' = e_m \setminus \{v_{m-1}\}$. Let $T' = (v_0, e_1, v_1, e_2, \dots, v_{m-1}, e, u, e', v_m)$. Obviously, $T' \cong P_n^{m+1}$.

As we pass from P_n^m to T', the distance between v_{m-1} and v_m is increased by 1, and the distance between any other vertex pair is increased or remains unchanged. Thus $DD(P_n^m) < DD(P_n^{m+1})$. ■

For $n \geq 3$, let $B_{n,i}$ be the tree of order n obtained from a path $P_{n-1} = v_0 v_1 \dots v_{n-2}$ by attaching a pendant edge $\{v_i, v\}$.

Theorem 9. *Among hypertrees on n vertices,*

- $\dfrac{n(n-1)(2n-1)}{3}$ *for $n \geq 2$ is the largest degree distance, achieved uniquely by $P_{n,2}$;*
- 6 *for $n = 3$ and* $\dfrac{2n^3 - 3n^2 - 11n + 36}{3}$ *for $n \geq 4$ are the second largest degree distance, achieved uniquely by $S_{3,3}$ and $B_{n,1}$, respectively;*
- 19 *for $n = 4$,* 45 *for $n = 5$ and* $\dfrac{2n^3 - 3n^2 - 23n + 96}{3}$ *for $n \geq 6$ are the third largest degree distances, achieved uniquely by P_4^2, P_5^3 and $B_{n,2}$, respectively.*

Proof. The result for $n = 2, 3$ is trivial, as there is only one hypertree $P_{2,2}$ on 2 vertices and there are exactly two hypertrees $P_{3,2}$ and $S_{3,3}$ on 3 vertices with $DD(S_{3,3}) = 6$.

Suppose $n \geq 4$. For convenience, let

$$\begin{aligned} f_1(n) &= \frac{n(n-1)(2n-1)}{3}, \\ f_2(n) &= \frac{2n^3 - 3n^2 - 11n + 36}{3}, \\ f_3(n) &= \frac{2n^3 - 3n^2 - 23n + 96}{3}, \\ g(n) &= \frac{4n^3 - 9n^2 - 7n + 30}{6}. \end{aligned}$$

Let T be a hypertree on n vertices with m edges, where $1 \leq m \leq n-1$. If $m \leq n-2$, then by Theorem 8, $DD(T) \leq DD(P_n^m)$ with equality if and only if $T \cong P_n^m$. By Lemma 5 and Theorem 8, $DD(P_n^m) \leq DD(P_n^{n-2}) = g(n)$. If $m = n-1$, then T is an ordinary tree, and thus we have either $T \cong P_{n,2}, B_{n,1}$ with

$$DD(P_{n,2}) = f_1(n) > DD(B_{n,1}) = f_2(n).$$

or $DD(T) \leq f_3(n)$ with equality if and only if $T \cong B_{n,2}$.

If $n \geq 6$, then $T \cong P_{n,2}, B_{n,1}$ or

$$DD(T) \leq \max\{DD(P_n^{n-2}), DD(B_{n,2})\} = \max\{g(n), f_3(n)\}.$$

Note that $g(n) < f_3(n) < f_2(n) < f_1(n)$ for $n \geq 6$. Thus, the result follows if $n \geq 6$.

If $n = 4, 5$, then $T \cong P_{n,2}, B_{n,1}$ or $DD(T) \leq DD(P_n^2) = g(n)$ with equality if and only if $T \cong P_n^{n-2}$. Note that $g(n) < f_2(n) < f_1(n)$ for $n = 4, 5$ and $g(4) = 19$ and $g(5) = 45$. Thus, the result follows if $n = 4, 5$. ■

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References

[1] P. Ali, S. Mukwembi, S. Munyira, Degree distance and vertex-connectivity, *Discr. Appl. Math.* **161** (2013) 2802–2811.

[2] P. Dankelmann, I. Gutman, S. Mukwembi, H. C. Swart, On the degree distance of a graph, *Discr. Appl. Math.* **157** (2009) 2773–2777.

[3] K. C. Das, I. Gutman, Estimating the Wiener index by means of number of vertices, number of edges, and diameter, *MATCH Commun. Math. Comput. Chem.* **64** (2010) 647–660.

[4] A. A. Dobrynin, R. Entringer, I. Gutman, Wiener index of trees: theory and applications, *Acta Appl. Math.* **66** (2001) 211–249.

[5] A. A. Dobrynin, I. Gutman, S. Klavžar, R. Žigert, Wiener index of hexagonal systems, *Acta Appl. Math.* **72** (2002) 247–294.

[6] A. A. Dobrynin, A. A. Kochetova, Degree distance of a graph: a degree analogue of the Wiener index, *J. Chem. Inf. Comput. Sci.* **34** (1994) 1082–1086.

[7] Z. Du, B. Zhou, Degree distance of unicyclic graphs, *Filomat* **24** (2010) 95–120.

[8] Z. Du, B. Zhou, Maximum degree distance of graphs with exactly two cycles, *Bull. Math. Soc. Sci. Math. Roumanie (N.S.)* **54** (2011) 119–136.

[9] B. Furtula, I. Gutman, H. Lin, More trees with all degrees odd having extremal Wiener index, *MATCH Commun. Math. Comput. Chem.* **70** (2013) 293–296.

[10] H. Guo, B. Zhou, Properties of degree distance and Gutman index of uniform hypergraphs, *MATCH Commun. Math. Comput. Chem.* **78** (2017) 213–220.

[11] H. Guo, B. Zhou, H. Lin, The Wiener index of uniform hypergraphs, *MATCH Commun. Math. Comput. Chem.* **78** (2017) 133–152.

[12] I. Gutman, Selected properties of the Schultz molecular topological index, *J. Chem. Inf. Comput. Sci.* **34** (1994) 1087–1089.

[13] I. Gutman, R. Cruz, J. Rada, Wiener index of Eulerian graphs, *Discr. Appl. Math.* **162** (2014) 247–250.

[14] I. Gutman, E. V. Konstantinova, V. A. Skorobogatov, Molecular hypergraphs and Clar structural formulas of benzenoid hydrocarbons, *ACH Models Chem.* **136** (1999) 539–548.

[15] P. J. Hansen, J. P. Jurs, Chemical applications of graph theory. Part I. Fundamentals and topological indices, *J. Chem. Educ.* **65** (1988) 574–580.

[16] S. Kanwal, I. Tomescu, Bounds for degree distance of a graph, *Math. Rep. (Bucur.)* **17** (2015) 337–344.

[17] S. Klavžar, I. Gutman, A comparison of the Schultz molecular topological index with the Wiener index, *J. Chem. Inf. Comput. Sci.* **36** (1996) 1001–1003.

[18] D. Klein, Z. Mihalić, D. Plavšić, N. Trinajstić, Molecular topological index: a relation with the Wiener index, *J. Chem. Inf. Comput. Sci.* **32** (1992) 304–305.

[19] E. V. Konstantinova, *Chemical Hypergraph Theory*, Com^{2}MaC, Pohang Univ. Sci. Technology, Pohang, 2001.

[20] E. V. Konstantinova, V. A. Skoroboratov, Graph and hypergraph models of molecular structure: A comparative analysis of indices, *J. Struct. Chem.* **39** (1998) 958–966.

[21] E. V. Konstantinova, V. A. Skorobogatov, Application of hypergraph theory in chemistry, *Discr. Math.* **235** (2001) 365–383.

[22] S. Mukwembi, S. Munyira, Degree distance and minimum degree, *Bull. Austral. Math. Soc.* **87** (2013) 255–271.

[23] D. H. Rouvray, The rich legacy of half a century of the Wiener index, in: D. H. Rouvray, R. B. King (Eds.), *Topology in Chemistry: Discrete Mathematics of Molecules*, Horwood, Chichester, 2002, pp. 16–37.

[24] H. P. Schultz, Topological organic chemistry. 1. Graph theory and topological indices of alkanes, *J. Chem. Inf. Comput. Sci.* **29** (1989) 239–257.

[25] I. Tomescu, Some extremal properties of the degree distance of a graph, *Discr. Appl. Math.* **98** (1999) 159–163.

[26] I. Tomescu, Properties of connected graphs having minimum degree distance, *Discr. Appl. Math.* **309** (2008) 2745–2748.

[27] H. Wiener, Structural determination of paraffin boiling points, *J. Am. Chem. Soc.* **69** (1947) 17–20.