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The Wiener Index of Uniform Hypergraphs

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Abstract

The Wiener index of a connected hypergraph is defined as the summation of distances between all pairs of vertices. We determine the unique k-uniform hypertrees with maximum, second maximum and third maximum Wiener indices, as well as the unique k-uniform hypertrees with minimum, second minimum and third minimum Wiener indices, respectively. We also determine the unique hypertree with maximum Wiener index among k-uniform hypertrees with given maximum degree and study two types of graft transformations that increase the Wiener index.

1 Introduction

A hypergraph G consists of a vertex set $V(G)$ and an edge $E(G)$, where $V(G)$ is nonempty, and each edge $e \in E(G)$ is a nonempty subset of $V(G)$. For an integer $k \geq 2$, we say that a hypergraph G is k-uniform if every edge contains exactly k vertices. A (simple) graph is a 2-uniform hypergraph. The degree of a vertex v in G, denoted by $d_G(v)$, is the number of edges of G which contain v.

Hypergraph theory found applications in chemistry [4, 7, 8]. The study in [7] 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.

For $u, v \in V(G)$, a path from u to v in G is defined to be a 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 $v_{i-1}, v_i \in e_i$ for $i = 1, \ldots, p$, where $v_0 = u$ and $v_p = v$. A cycle in G is defined to be a 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

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all e_i distinct such that $v_{i-1}, v_i \in e_i$ for $i = 1, \ldots, p$. The value p is the length of this path or cycle. If there is a path from u to v for any $u, v \in V(G)$, then we say that G is connected.

Let G be a k-uniform hypergraph with $V(G) = \{v_1, \ldots, v_n\}$. 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 Wiener index $W(G)$ of G is defined as the summation of distances between all unordered pairs of distinct vertices in G, i.e., $W(G) = \sum_{\{u,v\} \subseteq V(G)} d_G(u, v)$. Let $W_G(u) = \sum_{v \in V(G)} d_G(u, v)$. Then $W(G) = \frac{1}{2} \sum_{u \in V(G)} W_G(u)$.

The Wiener index of an ordinary (connected) graph has a long history [2, 5, 11, 13, 14] since 1947 when Wiener introduced this parameter as the path number [16]. The empirical Wiener's definition has been formalized via the distance matrix by Hosoya [6]. The study of transmission [12], average distance [1], and mean distance [3] of a connected graph is essentially the study of Wiener index. The Wiener index of a (connected) hypergraph was discussed in [9]. In a very recent paper, Sun et al. [15] computed the Wiener indices of some special k-uniform hypergraphs, and provided a lower bound for Wiener index of a k-uniform hypergraph with given circumference.

A hypertree is a connected hypergraph with no cycle. A k-uniform hypertree with m edges always has $1 + (k-1)m$ vertices.

In this paper, we determine the unique k-uniform hypertrees with maximum, second maximum and third maximum Wiener indices, as well as the unique k-uniform hypertrees with minimum, second minimum and third minimum Wiener indices, respectively and we also determine the unique hypertree with maximum Wiener index among k-uniform hypertrees with given maximum degree, and study two types of graft transformations that increase the Wiener index.

2 Preliminaries

Let G be a connected hypergraph. For $A \subseteq V(G)$, let $W_G(A) = \sum_{\{u,v\} \subseteq A} d_G(u, v)$. For $A, B \subseteq V(G)$ with $A \cap B = \emptyset$, let $W_G(A, B) = \sum_{a \in A, b \in B} d_G(a, b)$.

For $u \in V(G)$, let $G - u$ be the sub-hypergraph of G obtained by deleting u and all edges containing u. We remark that in the literature this is sometimes denoted by strongly deleting the vertex u. For $e \in E(G)$, let $G - e$ be the sub-hypergraph of G obtained by deleting e. For $X \subseteq V(G)$ with $X \neq \varnothing$, let $G[X]$ be the sub-hypergraph induced by X, i.e., $G[X]$ has vertex set X and edge set $\{e \subseteq X : e \in E(G)\}$.

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 $d_G(w_1) \geq 2$, $d_G(w_i) = 1$ for $2 \leq i \leq k$. A vertex of degree one is known as a pendant vertex.

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 with $H = G[V(G) \setminus (V(P) \setminus \{u\})]$. 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 G be a k-uniform hypergraph with $u, v \in V(G)$ and $e_1, \ldots, e_r \in E(G)$ such that $u \in e_i$, $v \notin e_i$ and $e_i' \notin E(G)$ for $1 \leq i \leq r$, where $e_i' = (e_i \setminus \{u\}) \cup \{v\}$. 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 u to v.

3 Hypergraph transformations increasing Wiener index

In the following, we propose two types of graft transformations that increase the Wiener index.

Let G be a connected k-uniform hypergraph with $u, v \in e \in E(G)$. For nonnegative integers p and q, let $G_{u,v}(p, q)$ be the k-uniform hypergraph obtained from G by attaching a pendant path of length p at u and a pendant path of length q at v.

Proposition 3.1. *Let G be a connected k-uniform hypergraph with $|E(G)| \geq 2$, $u, v \in e \in E(G)$ and $d_G(u) = 1$. For integers $p \geq q \geq 1$, $W(G_{u,v}(p, q)) < W(G_{u,v}(p+1, q-1))$.*

Proof. Let $H = G_{u,v}(p, q)$. Let $P = (u, e_1, u_1, \ldots, u_{p-1}, e_p, u_p)$ and $Q = (v, e_1', v_1, \ldots, v_{q-1}, e_q', v_q)$ be the pendant paths of H at u and v of lengths p and q, respectively.

Let H^* be the hypergraph obtained from H by moving edge e_q' from v_{q-1} to u_p. It is easily seen that $H^* \cong G_{u,v}(p+1, q-1)$. Let $V_1 = e \cup V(P) \cup (V(Q) \setminus (e_q' \setminus \{v_{q-1}\}))$. Note that

$$
\begin{aligned}
W_H(V(H) \setminus (e_q' \setminus \{v_{q-1}\})) &= W_{H^*}(V(H) \setminus (e_q' \setminus \{v_{q-1}\})), \\
W_H(e_q' \setminus \{v_{q-1}\}) &= W_{H^*}(e_q' \setminus \{v_{q-1}\}), \\
W_H(e_q' \setminus \{v_{q-1}\}, V_1) &= W_{H^*}(e_q' \setminus \{v_{q-1}\}, V_1),
\end{aligned}
$$

and

$$W_H(e'_q \setminus \{v_{q-1}\}, V(H) \setminus V_1) < W_{H^*}(e'_q \setminus \{v_{q-1}\}, V(H) \setminus V_1).$$

The only inequality holds because as we pass from H to H^*, the distance between a vertex of $e'_q \setminus \{v_{q-1}\}$ and a vertex of $V(H) \setminus V_1$ is increased by at least 1, which follows from the fact that $d_G(u) = 1$. Since

$$\begin{aligned} W(H) &= W_H(V(H) \setminus (e'_q \setminus \{v_{q-1}\})) + W_H(e'_q \setminus \{v_{q-1}\}) \\ &\quad + W_H(e'_q \setminus \{v_{q-1}\}, V_1) + W_H(e'_q \setminus \{v_{q-1}\}, V(H) \setminus V_1) \end{aligned}$$

and

$$\begin{aligned} W(H^*) &= W_{H^*}(V(H) \setminus (e'_q \setminus \{v_{q-1}\})) + W_{H^*}(e'_q \setminus \{v_{q-1}\}) \\ &\quad + W_{H^*}(e'_q \setminus \{v_{q-1}\}, V_1) + W_{H^*}(e'_q \setminus \{v_{q-1}\}, V(H) \setminus V_1), \end{aligned}$$

we have

$$W(H) - W(H^*) = W_H(e'_q \setminus \{v_{q-1}\}, V(H) \setminus V_1) - W_{H^*}(e'_q \setminus \{v_{q-1}\}, V(H) \setminus V_1) < 0,$$

i.e., $W(H) < W(H^*)$. ■

For positive integers p, q, and a k-uniform hypergraph G, let $G_u(p,q)$ be the k-uniform hypergraph obtained from G by attaching two pendant paths of lengths p and q at u, respectively, and $G_u(p,0)$ be the k-uniform hypergraph obtained from G by attaching a pendant path of length p at u.

Proposition 3.2. *Let G be a connected k-uniform hypergraph with $|E(G)| \geq 1$ and $u \in V(G)$. For integers $p \geq q \geq 1$, $W(G_u(p,q)) < W(G_u(p+1, q-1))$.*

Proof. Let $H = G_u(p,q)$. Let $P = (u, e_1, u_1, \ldots, u_{p-1}, e_p, u_p)$ and $Q = (u, e'_1, v_1, \ldots, v_{q-1}, e'_q, v_q)$ be the pendant paths of H at u of lengths p and q, respectively.

Let H^* be the hypergraph obtained from H by moving edge e'_q from v_{q-1} to u_p. It is easily seen that $H^* \cong G_u(p+1, q-1)$. Let $V_1 = V(P) \cup (V(Q) \setminus (e'_q \setminus \{v_{q-1}\}))$. Note that

$$\begin{aligned} W_H(V(H) \setminus (e'_q \setminus \{v_{q-1}\})) &= W_{H^*}(V(H) \setminus (e'_q \setminus \{v_{q-1}\})), \\ W_H(e'_q \setminus \{v_{q-1}\}) &= W_{H^*}(e'_q \setminus \{v_{q-1}\}), \\ W_H(e'_q \setminus \{v_{q-1}\}, V_1) &= W_{H^*}(e'_q \setminus \{v_{q-1}\}, V_1), \end{aligned}$$

and

$$W_H(e'_q \setminus \{v_{q-1}\}, V(H) \setminus V_1) < W_{H^*}(e'_q \setminus \{v_{q-1}\}, V(H) \setminus V_1).$$

The only inequality holds because as we pass from H to H^*, the distance between a vertex of $e'_q \setminus \{v_{q-1}\}$ and a vertex of $V(H) \setminus V_1$ is increased by at least 1. Since

$$\begin{aligned} W(H) &= W_H(V(H) \setminus (e'_q \setminus \{v_{q-1}\})) + W_H(e'_q \setminus \{v_{q-1}\}) \\ &\quad + W_H(e'_q \setminus \{v_{q-1}\}, V_1) + W_H(e'_q \setminus \{v_{q-1}\}, V(H) \setminus V_1) \end{aligned}$$

and

$$\begin{aligned} W(H^*) &= W_{H^*}(V(H) \setminus (e'_q \setminus \{v_{q-1}\})) + W_{H^*}(e'_q \setminus \{v_{q-1}\}) \\ &\quad + W_{H^*}(e'_q \setminus \{v_{q-1}\}, V_1) + W_{H^*}(e'_q \setminus \{v_{q-1}\}, V(H) \setminus V_1), \end{aligned}$$

we have

$$W(H) - W(H^*) = W_H(e'_q \setminus \{v_{q-1}\}, V(H) \setminus V_1) - W_{H^*}(e'_q \setminus \{v_{q-1}\}, V(H) \setminus V_1) < 0,$$

i.e., $W(H) < W(H^*)$. ■

For a k-uniform hypertree G with $V(G) = \{v_1, \ldots, v_n\}$, if $E(G) = \{e_1, \ldots, e_m\}$, 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 $P_{n,k}$.

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

For positive integers Δ, n with $1 \le \Delta \le \frac{n-1}{k-1}$, let $B^{\Delta}_{n,k}$ be the k-uniform hypertree obtained from vertex-disjoint hyperstar $S_{(\Delta-1)(k-1)+1,k}$ with center u and loose path $P_{n-(\Delta-1)(k-1),k}$ with an end vertex v by identifying u and v. In particular, $B^{\Delta}_{n,k} \cong P_{n,k}$ if $\Delta = 1, 2$.

In the proof of the following theorem, we follow the proof given in [10].

Theorem 3.1. *Let T be a k-uniform hypertree on n vertices with maximum degree Δ, where $1 \le \Delta \le \frac{n-1}{k-1}$. Then $W(T) \le W(B^{\Delta}_{n,k})$ with equality if and only if $T \cong B^{\Delta}_{n,k}$.*

Proof. It is trivial if $\Delta = 1$. Suppose that $\Delta \ge 2$. Let T be a k-uniform hypertree on n vertices with maximum degree Δ having maximum Wiener index.

Let u be a vertex of T with degree Δ.

Case 1. $\Delta \ge 3$.

Suppose that there are at least two vertices of degree at least 3 in T. Choose a vertex v of degree at least 3 such that $d_T(u,v)$ is as large as possible. Let $T_1,\dots,T_{d_T(v)}$ be the vertex disjoint sub-hypergraphs of $T-v$ with $\cup_{i=1}^{d_T(v)}V(T_i)=V(T)\setminus\{v\}$ such that $T[V(T_i)\cup\{v\}]$ is a k-uniform hypertree for $1\le i\le d_T(v)$. Suppose without loss of generality that $u\in V(T_1)$. If $k=2$, then $T[V(T_i)\cup\{v\}]$ is a pendant path at v for $2\le i\le d_T(v)$. Suppose that $k\ge 3$ and $T[V(T_i)\cup\{v\}]$ is not a pendant path at v for $2\le i\le d_T(v)$. Then there is at least one edge in $T[V(T_i)\cup\{v\}]$ with at least three vertices of degree 2. We choose such an edge $e=\{w_1,\dots,w_k\}$ by requiring that $d_T(v,w_1)$ is as large as possible, where $d_T(v,w_1)=d_T(v,w_j)-1$ for $2\le j\le k$. Then there are two pendant paths at different vertices of e, say P at w_s and Q at w_t, where $2\le s<t\le k$. Let p and q with $p,q\ge 1$ be the length of P and Q, respectively. Then $T\cong H_{w_s,w_t}(p,q)$ with $H=T[V(T)\setminus(V(P\cup Q)\setminus\{w_s,w_t\})]$. Note that $d_H(w_s)=d_H(w_t)=1$. Suppose without loss of generality that $p\ge q$. Obviously, $T'=H_{w_s,w_t}(p+1,q-1)$ is a k-uniform hypertree with maximum degree Δ. By Proposition 3.1, we have $W(T')>W(T)$, a contradiction. Thus $T[V(T_i)\cup\{v\}]$ is a pendant path at v for $2\le i\le d_T(v)$ when $k\ge 2$. Let l_i be the lengths of the pendant path $T[V(T_i)\cup\{v\}]$ at v, where $2\le i\le d_T(v)$ and $l_i\ge 1$. Suppose without loss of generality that $l_2\ge l_3$. Then $T=G_v(l_2,l_3)$, where $G=T[V(T)\setminus(V(T_2)\cup V(T_3))]$. Note that $T''=G_v(l_2+1,l_3-1)$ is a k-uniform hypertree with maximum degree Δ. By Proposition 3.2, $W(T'')>W(T)$, a contradiction. Thus u is the unique vertex of degree at least 3 in T.

Let $G_1,\dots,G_\Delta$ be the vertex disjoint sub-hypergraphs of $T-u$ with $\cup_{i=1}^{\Delta}V(G_i)=V(T)\setminus\{u\}$ such that $T[V(G_i)\cup\{u\}]$ is a connected k-uniform hypergraph for $1\le i\le\Delta$. By similar argument as above, $T[V(G_i)\cup\{u\}]$ is a pendant path at u for $1\le i\le\Delta$. Suppose that there are at least two pendant paths of length at least 2 at u, say $T[V(G_i)\cup\{u\}]$ and $T[V(G_j)\cup\{u\}]$ are such two paths with lengths p and q respectively, where $1\le i<j\le\Delta$. Then $T\cong H_u(p,q)$ with $H=T[V(T)\setminus(V(G_i)\cup V(G_j))]$. Suppose without loss of generality that $p\ge q$. Then $T'=H_u(p+1,q-1)$ is a k-uniform hypertree with maximum degree Δ. By Proposition 3.2, we have $W(T')>W(T)$, a contradiction. Thus there is at most one pendant path of length at least 1, implying that $T\cong B_{n,k}^{\Delta}$.

Case 2. $\Delta=2$.

It is trivial if $k=2$. Suppose that $k\ge 3$ and $T\ncong B_{n,k}^2$. Then there is an edge in T with at least three vertices of degree 2. We choose such an edge $e=\{w_1,\dots,w_k\}$ in T by requiring that $d_T(u,w_1)$ is as large as possible, where $d_T(u,w_1)=d_T(u,w_j)-1$ for

$2 \leq j \leq k$. Then there are two pendant paths at different vertices of e, say P at w_j and Q at w_l, where $2 \leq j < l \leq k$. Let p and q with $p, q \geq 1$ be the lengths of P and Q, respectively. Then $T \cong H_{w_j,w_l}(p,q)$ with $H = T[V(T) \setminus (V(P \cup Q) \setminus \{w_j, w_l\})]$. Note that $d_H(w_j) = d_H(w_l) = 1$. Suppose without loss of generality that $p \geq q$. Obviously, $T' = H_{w_j,w_l}(p+1, q-1)$ is a k-uniform hypertree with maximum degree 2. By Proposition 3.1, we have $W(T') > W(T)$, a contradiction. Thus there are at most two vertices of degree 2 in each edge, implying that $T \cong B^2_{n,k}$.

Combining Cases 1 and 2, we complete the proof. ∎

4 Hypertrees with large Wiener indices

In this section, we determine the unique k-uniform hypertrees with maximum, second maximum and third maximum Wiener indices, respectively.

Theorem 4.1. *For $\frac{n-1}{k-1} \geq 1$, let T be a k-uniform hypertree on n vertices. Then $W(T) \leq W(P_{n,k})$ with equality if and only if $T \cong P_{n,k}$.*

Proof. It is trivial if $\frac{n-1}{k-1} = 1, 2$. Suppose that $\frac{n-1}{k-1} \geq 3$. Let T be a k-uniform hypertree on n vertices with maximum Wiener index. Let Δ be the maximum degree of T. Then by Theorem 3.1, $T \cong B^{\Delta}_{n,k}$. Suppose that $\Delta \geq 3$. Then by Proposition 3.2, we have $W(B^{\Delta}_{n,k}) < W(B^{\Delta-1}_{n,k})$, a contradiction. Then $\Delta = 2$, and thus $T \cong B^2_{n,k} \cong P_{n,k}$. ∎

For $k \geq 3$, $\frac{n-1}{k-1} \geq 3$ and a loose path $P_{n-k+1,k} = \left(u_0, e_1, u_1, \ldots, e_{\frac{n-k}{k-1}}, u_{\frac{n-k}{k-1}}\right)$, let $F_{n,k}$ be the k-uniform hypertree obtained from $P_{n-k+1,k}$ by attaching a pendant edge at a vertex in $e_2 \setminus \{u_1, u_2\}$. If $\frac{n-1}{k-1} = 3$, then $F_{n,k} \cong P_{n,k}$. Let $F_{n,2} = B^3_{n,2}$.

Lemma 4.1. *Suppose that $k \geq 3$ and $\frac{n-1}{k-1} \geq 3$. Then $W(B^3_{n,k}) < W(F_{n,k})$.*

Proof. If $\frac{n-1}{k-1} = 3$, then the result follows from Theorem 4.1. Suppose that $\frac{n-1}{k-1} \geq 4$. Let $T = F_{n,k}$. Let $v \in e_2 \setminus \{u_1, u_2\}$ with $d_T(v) = 2$, and let e be the pendant edge at v in T. Let T' be the hypergraph obtained from T by moving e from v to u_1. Obviously, $T' \cong B^3_{n,k}$. Let $V_1 = V(T) \setminus (e \setminus \{v\})$. Note that

$$\begin{aligned} W_T(V_1) &= W_{T'}(V_1), \\ W_T(e \setminus \{v\}) &= W_{T'}(e \setminus \{v\}), \\ W_T(e \setminus \{v\}, V_1 \setminus (e_1 \setminus \{u_1\})) &= W_{T'}(e \setminus \{v\}, V_1 \setminus (e_1 \setminus \{u_1\})), \end{aligned}$$

and

$$W_T(e \setminus \{v\}, e_1 \setminus \{u_1\}) > W_{T'}(e \setminus \{v\}, e_1 \setminus \{u_1\}).$$

The only inequality holds because as we pass from T to T', the distance between a vertex of $e \setminus \{v\}$ and a vertex of $e_1 \setminus \{u_1\}$ is decreased by 1. Since

$$\begin{aligned} W(T) &= W_T(V_1) + W_T(e \setminus \{v\}) + W_T(e \setminus \{v\}, V_1 \setminus (e_1 \setminus \{u_1\})) \\ &\quad + W_T(e \setminus \{v\}, e_1 \setminus \{u_1\}) \end{aligned}$$

and

$$\begin{aligned} W(T') &= W_{T'}(V_1) + W_{T'}(e \setminus \{v\}) + W_{T'}(e \setminus \{v\}, V_1 \setminus (e \setminus \{u_1\})) \\ &\quad + W_{T'}(e \setminus \{v\}, e_1 \setminus \{u_1\}), \end{aligned}$$

we have

$$W(T) - W(T') = W_T(e \setminus \{v\}, e_1 \setminus \{u_1\}) - W_{T'}(e \setminus \{v\}, e_1 \setminus \{u_1\}) > 0,$$

i.e., $W(T') < W(T)$. ■

Theorem 4.2. *For $\frac{n-1}{k-1} \geq 4$, let T be a k-uniform hypertree with n vertices. Suppose that $T \ncong P_{n,k}$. Then $W(T) \leq W(F_{n,k})$ with equality if and only if $T \cong F_{n,k}$.*

Proof. Let T be a k-uniform hypertree on n vertices nonisomorphic to $P_{n,k}$ with maximum Wiener index.

Let Δ be the maximum degree of T. Then $\Delta \geq 3$ if $k = 2$ and $\Delta \geq 2$ if $k \geq 3$.

If $\Delta \geq 3$, then by Theorem 3.1, $T \cong B^{\Delta}_{n,k}$. Suppose that $\Delta \geq 4$. Note that $B^{\Delta-1}_{n,k} \ncong P_{n,k}$. By Proposition 3.2, we have $W(T) = W(B^{\Delta}_{n,k}) < W(B^{\Delta-1}_{n,k})$, a contradiction. Thus $\Delta = 2$ or 3, and if $\Delta = 3$, then $T \cong B^{3}_{n,k}$.

Suppose that $\Delta = 2$. Then $k \geq 3$. Since $T \ncong P_{n,k}$, there is at least one edge with at least three vertices of degree 2. Suppose that there are at least two such edges. Let u be a vertex of degree 1 in T. Choose an edge $e = \{w_1, \ldots, w_k\}$ in T with at least three vertices of degree 2 such that $d_T(u, w_1)$ is as large as possible, where $d_T(u, w_1) = d_T(u, w_i) - 1$ for $2 \leq i \leq k$. Then there are two pendant paths at different vertices of e, say P at w_i and Q at w_j, where $1 \leq i < j \leq k$. Let p and q with $p, q \geq 1$ be the lengths of P and Q, respectively. Then $T \cong H_{w_i,w_j}(p, q)$ with $H = T[V(T) \setminus (V(P \cup Q) \setminus \{w_i, w_j\})]$. Note that $d_H(w_i) = d_H(w_j) = 1$. Suppose without loss of generality that $p \geq q$. Obviously, $T' = H_{w_i,w_j}(p + 1, q - 1)$ is a k-uniform hypertree that is not isomorphic to $P_{n,k}$. By Proposition 3.1, we have $W(T) < W(T')$, a contradiction. Thus e is the unique edge with at least three vertices of degree 2.

Suppose that there are four vertices, say w_1, w_2, w_3 and w_4 of degree 2 in e. Let Q_i be the pendant path of length l_i at w_i, where $l_i \geq 1$ for $i = 1, 2, 3, 4$. Suppose without loss of generality that $l_1 \geq l_2$. Let $G = T[V(T)\setminus(V(Q_1 \cup Q_2)\setminus\{w_1, w_2\})]$. Then $T \cong G_{w_1,w_2}(l_1, l_2)$. Note that $d_G(w_1) = 1$ and $T'' = G_{w_1,w_2}(l_1 + 1, l_2 - 1)$ is a k-uniform hypertree that is not isomorphic to $P_{n,k}$. By Proposition 3.1, $W(T) < W(T'')$, a contradiction. Thus there are exactly three vertices of degree 2 in e, say w_1, w_2, and w_3.

Let Q_i be the pendant path at w_i with length l_i, where $i = 1, 2, 3$ and $l_i \geq 1$. Suppose without loss of generality that $l_1 \geq l_2 \geq l_3$. Suppose that $l_1 \geq l_2 \geq 2$. Let $G = T[V(T) \setminus (V(Q_1 \cup Q_2) \setminus \{w_1, w_2\})]$. Then $T \cong G_{w_1,w_2}(l_1, l_2)$. Note that $d_G(w_1) = 1$ and $T^* = G_{w_1,w_2}(l_1 + 1, l_2 - 1)$ is a k-uniform hypertree that is not isomorphic to $P_{n,k}$. By Proposition 3.1, $W(T) < W(T^*)$, a contradiction. Thus there are at least two of Q_1, Q_2 and Q_3 with length 1. It follows that $T \cong F_{n,k}$.

By Lemma 4.1, $W(B^3_{n,k}) < W(F_{n,k})$. Thus $T \cong F_{n,k}$. ■

For $k \geq 3$, $\frac{n-1}{k-1} \geq 5$ and a loose path $P_{n-k+1,k} = \left(u_0, e_1, u_1, \cdots, e_{\frac{n-k}{k-1}}, u_{\frac{n-k}{k-1}}\right)$, let $E_{n,k}$ be the k-uniform hypertree obtained from $P_{n-k+1,k}$ by attaching a pendant edge at a vertex in $e_3 \setminus \{u_2, u_3\}$.

Lemma 4.2. *Suppose that $k \geq 3$ and $\frac{n-1}{k-1} \geq 6$. Then $W(B^3_{n,k}) \geq W(E_{n,k})$ with equality if and only if $\frac{n-1}{k-1} = 6$.*

Proof. Let $T = E_{n,k}$. Let $v \in e_3 \setminus \{u_2, u_3\}$ with $d_T(v) = 2$, and let e be the pendant edge at v in T. Let T' be the hypergraph obtained from T by moving e from v to u_1. Obviously, $T' \cong B^3_{n,k}$. Let $V_1 = V(T) \setminus (e \setminus \{v\})$. Note that

$$\begin{aligned} W_T(V_1) &= W_{T'}(V_1), \\ W_T(e \setminus \{v\}) &= W_{T'}(e \setminus \{v\}), \end{aligned}$$

and

$$W_T(e \setminus \{v\}, e_2 \cup e_3) = W_{T'}(e \setminus \{v\}, e_2 \cup e_3).$$

As we pass from T to T', the distance between a vertex of $e\setminus\{v\}$ and a vertex of $e_1\setminus\{u_1\}$ is decreased by 2, and the distance between a vertex of $e\setminus\{v\}$ and a vertex of $V_1\setminus(e_1\cup e_2\cup e_3)$ is increased by 1. Note also that $|V_1 \setminus (e_1 \cup e_2 \cup e_3)| = \left(\frac{n-1}{k-1} - 4\right)(k - 1)$. Then

$$\begin{aligned} W_T(e \setminus \{v\}, e_1 \setminus \{u_1\}) - W_{T'}(e \setminus \{v\}, e_1 \setminus \{u_1\}) &= 2|e \setminus \{v\}| \cdot |e_1 \setminus \{u_1\}| \\ &= 2(k - 1)^2, \end{aligned}$$

and

$$\begin{aligned}
& W_T(e \setminus \{v\}, V_1 \setminus (e_1 \cup e_2 \cup e_3)) - W_{T'}(e \setminus \{v\}, V_1 \setminus (e_1 \cup e_2 \cup e_3)) \\
= \; & -|e \setminus \{v\}| \cdot |V_1 \setminus (e_1 \cup e_2 \cup e_3)| = -\left(\frac{n-1}{k-1} - 4\right)(k-1)^2.
\end{aligned}$$

Since

$$\begin{aligned}
W(T) &= W_T(V_1) + W_T(e \setminus \{v\}) + W_T(e \setminus \{v\}, e_2 \cup e_3) \\
&\quad + W_T(e \setminus \{v\}, e_1 \setminus \{u_1\}) + W_T(e \setminus \{v\}, V_1 \setminus (e_1 \cup e_2 \cup e_3))
\end{aligned}$$

and

$$\begin{aligned}
W(T') &= W_{T'}(V_1) + W_{T'}(e \setminus \{v\}) + W_{T'}(e \setminus \{v\}, e_2 \cup e_3) \\
&\quad + W_{T'}(e \setminus \{v\}, e_1 \setminus \{u_1\}) + W_{T'}(e \setminus \{v\}, V_1 \setminus (e_1 \cup e_2 \cup e_3)),
\end{aligned}$$

we have

$$\begin{aligned}
W(T) - W(T') &= W_T(e \setminus \{v\}, e_1 \setminus \{u_1\}) + W_T(e \setminus \{v\}, V_1 \setminus (e_1 \cup e_2 \cup e_3)) \\
&\quad - W_{T'}(e \setminus \{v\}, e_1 \setminus \{u_1\}) - W_{T'}(e \setminus \{v\}, V_1 \setminus (e_1 \cup e_2 \cup e_3)) \\
&= \left(6 - \frac{n-1}{k-1}\right)(k-1)^2,
\end{aligned}$$

and thus the result follows. ■

Let $F'_{n,2}$ be the tree obtained by attaching a pendant edge at vertex v_3 of the path $v_1 \dots v_{n-1}$. Let $F^*_{n,2}$ be the tree obtained by attaching two pendant edges at v_1 and v_{n-4} of the path $v_1 \dots v_{n-4}$, respectively.

Theorem 4.3. *For $\frac{n-1}{k-1} \geq 6$, let T be a k-uniform hypertree on n vertices. Suppose that $T \ncong F_{n,k}, P_{n,k}$. Then*

(i) if $k = 2$, then $W(T) \leq W(F'_{n,2})$ with equality if and only if $T \cong F'_{n,2}$;

(ii) if $k \geq 3$ and $\frac{n-1}{k-1} = 6$, then $W(T) \leq W(B^3_{n,k}) = W(E_{n,k})$ with equality if and only if $T \cong B^3_{n,k}$ or $T \cong E_{n,k}$;

(iii) if $k \geq 3$ and $\frac{n-1}{k-1} > 6$, then $W(T) \leq W(B^3_{n,k})$ with equality if and only if $T \cong B^3_{n,k}$.

Proof. Let T be a k-uniform hypertree on n vertices nonisomorphic to $P_{n,k}$ and $F_{n,k}$ with maximum Wiener index.

Let Δ be the maximum degree of T. Obviously, $\Delta \geq 2$.

Suppose that $\Delta \geq 4$. Then by Theorem 3.1, $T \cong B^\Delta_{n,k}$. Note that $F'_{n,2} \ncong F_{n,k}, P_{n,k}$ for $k = 2$ and $B^{\Delta-1}_{n,k} \ncong F_{n,k}, P_{n,k}$ for $k \geq 3$. By Proposition 3.2, we have $W(T) = W(B^\Delta_{n,k}) <$

$W(F'_{n,2})$ if $k = 2$ and $W(T) = W(B^{\Delta}_{n,k}) < W(B^{\Delta-1}_{n,k})$ for $k \geq 3$, a contradiction. Thus $\Delta = 2$ or 3.

Suppose that $k = 2$. Then $\Delta = 3$. Note that $T \ncong F_{n,2}$, $P_{n,2}$. By similar argument of Case 1 in the proof of Theorem 3.1, there are at most two vertices of degree 3 in T. If there is a unique vertex of degree 3 in T, then by Proposition 3.2, T is obtainable by attaching a pendant edge at a internal vertex of a path on $n-1$ vertices, and thus $T \cong F'_{n,2}$. If there are exactly two vertices of degree 3 in T, then by Proposition 3.2, T is obtainable by attaching two pendant edges each at an internal vertex of a path on $n-2$ vertices, and thus $T \cong F^*_{n,2}$. By direct calculation, we have $W(F'_{n,2}) > W(F^*_{n,2})$. This proves (i).

Suppose in the following that $k \geq 3$. If $\Delta = 3$, then by Theorem 3.1, $T \cong B^3_{n,k}$.

Now suppose that $\Delta = 2$. Since $T \ncong P_{n,k}$, there is at least one edge with at least three vertices of degree 2 in T. Suppose that there are at least two such edges. Let u be a vertex of degree 1 in T. Choose an edge $e = \{w_1, \dots, w_k\}$ in T with at least three vertices of degree 2 such that $d_T(u, w_1)$ is as large as possible, where $d_T(u, w_1) = d_T(u, w_i) - 1$ for $2 \leq i \leq k$. Then there are two pendant paths at different vertices of e, say P at w_i and Q at w_j, where $1 \leq i < j \leq k$. Let p and q with $p, q \geq 1$ be the lengths of P and Q, respectively. Then $T \cong H_{w_i,w_j}(p, q)$ with $H = T[V(T) \setminus (V(P \cup Q) \setminus \{w_i, w_j\})]$. Note that $d_H(w_i) = d_H(w_j) = 1$. Suppose without loss of generality that $p \geq q$. Note that $T' = H_{w_i,w_j}(p+1, q-1)$ is a k-uniform hypertree that is not isomorphic to $P_{n,k}$. If $T' = H_{w_i,w_j}(p+1, q-1)$ is also not isomorphic to $F_{n,k}$, then by Proposition 3.1, we have $W(T) < W(T')$, a contradiction. Suppose that $T' = H_{w_i,w_j}(p+1, q-1) \cong F_{n,k}$. Then T is isomorphic to the k-uniform hypertree obtained from $P_{n-2(k-1),k} = \left(u_0, e_1, u_1, \dots, u_{\frac{n-1}{k-1}-3}, e_{\frac{n-1}{k-1}-2}, u_{\frac{n-1}{k-1}-2}\right)$ by attaching a pendant edge e' at a vertex w' in $e_2 \setminus \{u_1, u_2\}$ and attaching a pendant edge e'' at a vertex w'' in $e_i \setminus \{u_{i-1}, u_i\}$, where $3 \leq i \leq \frac{n-1}{k-1} - 3$. Suppose without loss of generality that T is such a hypertree. By moving edge e'' from w'' to u_0 in T, we get a k-uniform hypertree T''. Let L be the unique path in T from u_0 to w'' and $V_1 = V(T) \setminus (V(L) \cup e' \cup e'')$. Then

$$\begin{aligned}
W_T(V(T) \setminus (e'' \setminus \{w''\})) &= W_{T''}(V(T) \setminus (e'' \setminus \{w''\})),\\
W_T(e'' \setminus \{w''\}) &= W_{T''}(e'' \setminus \{w''\}),\\
W_T(e'' \setminus \{w''\}, V(L)) &= W_{T''}(e'' \setminus \{w''\}, V(L)),
\end{aligned}$$

$$W_T(e'' \setminus \{w''\}, e' \setminus \{w'\}) - W_{T''}(e'' \setminus \{w''\}, e' \setminus \{w'\}) = (i-3)(k-1)^2,$$

and

$$W_T(e''\setminus\{w''\},V_1)-W_{T''}(e''\setminus\{w''\},V_1)=-\left(\frac{n-1}{k-1}-i-2\right)(i-1)(k-1)^2.$$

The last two equalities hold because as we pass from T to T'', the distance between a vertex of $e''\setminus\{w''\}$ and a vertex of $e'\setminus\{w'\}$ is decreased by $i-3$, and the distance between a vertex of $e''\setminus\{w''\}$ and a vertex of V_1 is increased by $i-1$. Note that

$$\begin{aligned} W(T) &= W_T(V(T)\setminus(e''\setminus\{w''\}))+W_T(e''\setminus\{w''\})+W_T(e''\setminus\{w''\},V(L)) \\ &\quad +W_T(e''\setminus\{w''\},e'\setminus\{w'\})+W_T(e''\setminus\{w''\},V_1), \end{aligned}$$

and

$$\begin{aligned} W(T'') &= W_{T''}(V(T)\setminus(e''\setminus\{w''\}))+W_{T''}(e''\setminus\{w''\})+W_{T''}(e''\setminus\{w''\},V(L)) \\ &\quad +W_{T''}(e''\setminus\{w''\},e'\setminus\{w'\})+W_{T''}(e''\setminus\{w''\},V_1). \end{aligned}$$

Then

$$\begin{aligned} W(T)-W(T'') &= W_T(e''\setminus\{w''\},e'\setminus\{w'\})+W_T(e''\setminus\{w''\},V_1) \\ &\quad -W_{T''}(e''\setminus\{w''\},e'\setminus\{w'\})-W_{T''}(e''\setminus\{w''\},V_1) \\ &= (i-3)(k-1)^2-\left(\frac{n-1}{k-1}-i-2\right)(i-1)(k-1)^2 \\ &\le (i-3)(k-1)^2-(i-1)(k-1)^2<0\,, \end{aligned}$$

and thus $W(T'')>W(T)$, a contradiction. Thus e is the unique edge with at least three vertices of degree 2.

Suppose that there are four vertices w_1,w_2,w_3 and w_4 of degree 2 in e. Let Q_i be the pendant path of length l_i at w_i, where $l_i\ge 1$ for $i=1,2$. Suppose without loss of generality that $l_1\ge l_2$. Let $G=T[V(T)\setminus(V(Q_1\cup Q_2)\setminus\{w_1,w_2\})]$. Then $T\cong G_{w_1,w_2}(l_1,l_2)$. Note that $d_G(w_1)=1$ and $T^*=G_{w_1,w_2}(l_1+1,l_2-1)$ is a k-uniform hypertree that is not isomorphic to $P_{n,k}$. If T^* is also not isomorphic to $F_{n,k}$, by Proposition 3.1, $W(T)<W(T^*)$, a contradiction. If $T^*\cong F_{n,k}$, then T is isomorphic to the k-uniform hypertree obtained from $P_{n-2(k-1),k}=\left(u_0,e_1,u_1,\ldots,u_{\frac{n-1}{k-1}-3},e_{\frac{n-1}{k-1}-2},u_{\frac{n-1}{k-1}-2}\right)$ by attaching pendant edges e' and e'' at y and z in $e_2\setminus\{u_1,u_2\}$, respectively, where $y\ne z$. Note that $T\cong H_{y,z}(1,1)$ with $H=T[V(T)\setminus((e'\cup e'')\setminus\{y,z\})]$. Let $T^{**}=H_{y,z}(2,0)$. Note that $T^{**}\cong E_{n,k}$. By Proposition 3.1, we have $W(T^{**})>W(T)$, a contradiction. Thus there are exactly three vertices of degree 2 in e, say w_1,w_2 and w_3.

Let Q_i be the pendant path at w_i with length l_i, where $i = 1, 2, 3$ and $l_i \geq 1$. Suppose without loss of generality that $l_1 \geq l_2 \geq l_3 \geq 2$. Let $G = T[V(T)\setminus(V(Q_1 \cup Q_2)\setminus\{w_1, w_2\})]$. Then $T \cong G_{w_1,w_2}(l_1, l_2)$. Note that $d_G(w_1) = 1$ and $T^* = G_{w_1,w_2}(l_1+1, l_2-1)$ is a k-uniform hypertree that is not isomorphic to $P_{n,k}$ and $F_{n,k}$. By Proposition 3.1, $W(T) < W(T^*)$, a contradiction. Thus there is at least one of Q_1, Q_2 and Q_3 with length 1.

As above, T is a k-uniform hypergraph obtained from $P_{n-k+1,k} = \Big(v_0, e_1, v_1, \ldots, v_{\frac{n-1}{k-1}-2}, e_{\frac{n-1}{k-1}-1}, v_{\frac{n-1}{k-1}-1}\Big)$ by attaching a pendant edge to a vertex of $e_i \setminus \{v_{i-1}, v_i\}$ with $3 \leq i \leq \frac{n-1}{k-1} - 3$.

Suppose that $T \ncong E_{n,k}$. Then there is a pendant edge e^* at a vertex w in $e_i \setminus \{v_{i-1}, v_i\}$, where $4 \leq i \leq \frac{n-1}{k-1} - 4$. Since $T \ncong F_{n,k}$, it is trivial if $\frac{n-1}{k-1} = 6, 7$. Suppose that $\frac{n-1}{k-1} \geq 8$ in the following. By moving the pendant edge e^* from w to a vertex, say v in $e_3 \setminus \{v_2, v_3\}$, we get a k-uniform hypergraph T^*. Note that $T^* \cong E_{n,k}$. Let P' be the unique path from v to w and $V_2 = V(T) \setminus (V(P') \cup e_1 \cup e_2 \cup e^*)$. Then

$$\begin{aligned}
W_T(V(T) \setminus (e^* \setminus \{w\})) &= W_{T^*}(V(T) \setminus (e^* \setminus \{w\})), \\
W_T(e^* \setminus \{w\}) &= W_{T^*}(e^* \setminus \{w\}), \\
W_T(e^* \setminus \{w\}, V(P')) &= W_{T^*}(e^* \setminus \{w\}, V(P')),
\end{aligned}$$

$$W_T(e^* \setminus \{w\}, e_1 \cup (e_2 \setminus \{u_2\})) - W_{T^*}(e^* \setminus \{w\}, e_1 \cup (e_2 \setminus \{u_2\})) = 2(i-3)(k-1)^2,$$

and

$$W_T(e^* \setminus \{w\}, V_2) - W_{T^*}(e^* \setminus \{w\}, V_2) = -\left(\frac{n-1}{k-1} - i - 1\right)(i-3)(k-1)^2.$$

The last two equalities hold because as we pass from T to T^*, the distance between a vertex of $e^* \setminus \{w\}$ and a vertex of $e_1 \cup (e_2 \setminus \{u_2\})$ is decreased by $i - 3$, and the distance between a vertex of $e^* \setminus \{w\}$ and a vertex of V_2 is increased by $i - 3$. Note that

$$\begin{aligned}
W(T) = {} & W_T(V(T) \setminus (e^* \setminus \{w\})) + W_T(e^* \setminus \{w\}) + W_T(e^* \setminus \{w\}, V(P')) \\
& + W_T(e^* \setminus \{w\}, e_1 \cup (e_2 \setminus \{u_2\})) + W_T(e^* \setminus \{w\}, V_2)
\end{aligned}$$

and

$$\begin{aligned}
W(T^*) = {} & W_{T^*}(V(T) \setminus (e^* \setminus \{w\})) + W_{T^*}(e^* \setminus \{w\}) + W_{T^*}(e^* \setminus \{w\}, V(P')) \\
& + W_{T^*}(e^* \setminus \{w\}, e_1 \cup (e_2 \setminus \{u_2\})) + W_{T^*}(e^* \setminus \{w\}, V_2).
\end{aligned}$$

Then

$$W(T) - W(T^*) = W_T(e^* \setminus \{w\}, e_1 \cup (e_2 \setminus \{u_2\})) + W_T(e^* \setminus \{w\}, V_2)$$

$$
\begin{aligned}
& -W_{T^*}(e^* \setminus \{w\}, e_1 \cup (e_2 \setminus \{u_2\})) - W_{T^*}(e^* \setminus \{w\}, V_2) \\
= \; & 2(i-3)(k-1)^2 - \left(\frac{n-1}{k-1} - i - 1\right)(i-3)(k-1)^2 \\
= \; & \left(3 + i - \frac{n-1}{k-1}\right)(i-3)(k-1)^2 < 0\,,
\end{aligned}
$$

and thus $W(T^*) > W(T)$, a contradiction. Therefore $T \cong E_{n,k}$ if $\Delta = 2$.

Now we have proved that $T \cong B^3_{n,k}$ or $T \cong E_{n,k}$ if $k \geq 3$. Thus the results (ii) and (iii) follow from Lemma 4.2. ∎

5 Hypertrees with small Wiener indices

In this section, we determine the unique k-uniform hypertrees with minimum, second minimum and third minimum Wiener indices, respectively.

Theorem 5.1. *For $\frac{n-1}{k-1} \geq 1$, let T be a k-uniform hypertree with n vertices. Then $W(T) \geq W(S_{n,k})$ with equality if and only if $T \cong S_{n,k}$.*

Proof. It is trivial if $\frac{n-1}{k-1} \leq 2$. Suppose that $\frac{n-1}{k-1} \geq 3$. Let T be a k-uniform hypertree on n vertices with minimum Wiener index.

Let d be the diameter of T. Obviously, $d \geq 2$. Suppose that $d \geq 3$. Let $P = (v_0, e_1, v_1, \ldots, v_{d-1}, e_d, v_d)$ be a diametral path of T. Let E be the set of edges containing v_{d-1} except e_{d-1}, E_1 be the set of vertices in those edges in E, and $E_1' = E_1 \setminus \{v_{d-1}\}$. By moving each edge in E from v_{d-1} to v_{d-2} in T, we get a k-uniform hypertree T'. Let Q be the set of vertices in e_{d-1} and pendant edges at each vertex in $e_{d-1} \setminus \{v_{d-2}, v_{d-1}\}$. Let $V = V(T)$. Note that

$$
\begin{aligned}
W_T(E_1') &= W_{T'}(E_1'), \\
W_T(V \setminus E_1') &= W_{T'}(V \setminus E_1'), \\
W_T(E_1', Q) &= W_{T'}(E_1', Q),
\end{aligned}
$$

and

$$W_T(E_1', V \setminus (E_1' \cup Q)) > W_{T'}(E_1', V \setminus (E_1' \cup Q)).$$

The only inequality holds because as we pass from T to T', the distance between a vertex of E_1' and a vertex of $V \setminus (E_1' \cup Q)$ is decreased by 1. Since

$$W(T) \;=\; W_T(E_1') + W_T(V \setminus E_1') + W_T(E_1', Q) + W_T(E_1', V \setminus (E_1' \cup Q))$$

and

$$W(T') = W_{T'}(E_1') + W_{T'}(V \setminus E_1') + W_{T'}(E_1', Q) + W_{T'}(E_1', V \setminus (E_1' \cup Q)),$$

we have

$$W(T) - W(T') = W_T(E_1', V \setminus (E_1' \cup Q)) - W_{T'}(E_1', V \setminus (E_1' \cup Q)) > 0,$$

and thus $W(T') < W(T)$, a contradiction. Thus $d = 2$, implying that $T \cong S_{n,k}$. ∎

For $\frac{n-1}{k-1} \geq 3$ and $1 \leq a \leq \left\lfloor \frac{n-k}{2(k-1)} \right\rfloor$, let $D_{n,k,a}$ be the k-uniform hypertree obtained from vertex-disjoint $S_{a(k-1)+1,k}$ with center u and $S_{n-k-a(k-1)+1,k}$ with center v by adding $k-2$ new vertices $w_1, \ldots, w_{k-2}$ and an edge $\{u, v, w_1, \ldots, w_{k-2}\}$.

Lemma 5.1. *For $2 \leq a \leq \left\lfloor \frac{n-k}{2(k-1)} \right\rfloor$, $W(D_{n,k,a}) > W(D_{n,k,a-1})$.*

Proof. Let $b = \frac{n-k}{k-1} - a$. Let u and v be the vertices of $D_{n,k,a}$ with degrees $a+1$ and $b+1$, respectively. Let $E(D_{n,k,a}) = E(u) \cup E(v) \cup e$, where $e = \{u, v, w_1, \ldots, w_{k-2}\}$, and $E(u), E(v)$ are respectively the set of edges containing u, v except e. Let $E_1(u)$ and $E_1(v)$ be the set of vertices in those edges of $E(u)$ and $E(v)$, respectively. By moving an edge $e' \in E(u)$ from u to v, we get $D_{n,k,a-1}$. Let $V = V(D_{n,k,a})$. Note that

$$\begin{aligned} W_{D_{n,k,a}}(e' \setminus \{u\}) &= W_{D_{n,k,a-1}}(e' \setminus \{u\}), \\ W_{D_{n,k,a}}(V \setminus (e' \setminus \{u\})) &= W_{D_{n,k,a-1}}(V \setminus (e' \setminus \{u\})), \\ W_{D_{n,k,a}}(e' \setminus \{u\}, e) &= W_{D_{n,k,a-1}}(e' \setminus \{u\}, e), \end{aligned}$$

$$W_{D_{n,k,a}}(e' \setminus \{u\}, E_1(v) \setminus \{v\}) - W_{D_{n,k,a-1}}(e' \setminus \{u\}, E_1(v) \setminus \{v\}) = b(k-1)^2,$$

and

$$W_{D_{n,k,a}}(e' \setminus \{u\}, E_1(u) \setminus e') - W_{D_{n,k,a-1}}(e' \setminus \{u\}, E_1(u) \setminus e') = -(a-1)(k-1)^2.$$

The last two equalities hold because as we pass from $D_{n,k,a}$ to $D_{n,k,a-1}$, the distance between a vertex of $e' \setminus \{u\}$ and a vertex of $E_1(v) \setminus \{v\}$ is decreased by 1, and the distance between a vertex of $e' \setminus \{u\}$ and a vertex of $E_1(u) \setminus e'$ is increased by 1. Since

$$\begin{aligned} W(D_{n,k,a}) = {} & W_{D_{n,k,a}}(e' \setminus \{u\}) + W_{D_{n,k,a}}(V \setminus (e' \setminus \{u\})) + W_{D_{n,k,a}}(e' \setminus \{u\}, e) \\ & + W_{D_{n,k,a}}(e' \setminus \{u\}, E_1(v) \setminus \{v\}) + W_{D_{n,k,a}}(e' \setminus \{u\}, E_1(u) \setminus e') \end{aligned}$$

and

$$W(D_{n,k,a-1}) = W_{D_{n,k,a-1}}(e' \setminus \{u\}) + W_{D_{n,k,a-1}}(V \setminus (e' \setminus \{u\})) + W_{D_{n,k,a-1}}(e' \setminus \{u\}, e)$$

$$+W_{D_{n,k,a-1}}(e' \setminus \{u\}, E_1(v) \setminus \{v\}) + W_{D_{n,k,a-1}}(e' \setminus \{u\}, E_1(u) \setminus e'),$$

we have

$$\begin{aligned}
& W(D_{n,k,a}) - W(D_{n,k,a-1}) \\
= \ & W_{D_{n,k,a}}(e' \setminus \{u\}, E_1(v) \setminus \{v\}) + W_{D_{n,k,a}}(e' \setminus \{u\}, E_1(u) \setminus e') \\
& -W_{D_{n,k,a-1}}(e' \setminus \{u\}, E_1(v) \setminus \{v\}) - W_{D_{n,k,a-1}}(e' \setminus \{u\}, E_1(u) \setminus e') \\
= \ & b(k-1)^2 - (a-1)(k-1)^2 > 0\,,
\end{aligned}$$

and thus $W(D_{n,k,a}) > W(D_{n,k,a-1})$. ■

Theorem 5.2. *For $\frac{n-1}{k-1} \geq 3$, let T be a k-uniform hypertree on n vertices. Suppose that $T \ncong S_{n,k}$. Then $W(T) \geq W(D_{n,k,1})$ with equality if and only if $T \cong D_{n,k,1}$.*

Proof. It is trivial if $\frac{n-1}{k-1} = 3$. Suppose that $\frac{n-1}{k-1} \geq 4$. Let T be a k-uniform hypertree on n vertices nonisomorphic to $S_{n,k}$ with minimum Wiener index.

Let d be the diameter of T. Since $T \ncong S_{n,k}$, we have $d \geq 3$. By similar argument as in the proof of Theorem 5.1, we have $d = 3$. Let $P = (v_0, e_1, v_1, e_2, v_2, e_3, v_3)$ be a diametral path of T, and $V = V(T)$.

Suppose that $k \geq 3$ and there is at least one pendant edge at a vertex $u \in e_2 \setminus \{v_1, v_2\}$. For $w \in \{u, v_2\}$, let $E(w)$ be the set of edges containing w except e_2, $E_1(w)$ be the set of vertices in those edges in $E(w)$, and $E'_1(w) = E_1(w) \setminus \{w\}$. By moving each edge in $E(u)$ from u to v_2 in T, we get a k-uniform hypertree T'. Obviously, $T' \ncong S_{n,k}$. Note that

$$\begin{aligned}
W_T(V \setminus E'_1(u)) &= W_{T'}(V \setminus E'_1(u)), \\
W_T(E'_1(u)) &= W_{T'}(E'_1(u)), \\
W_T(E'_1(u), V \setminus (E'_1(u) \cup E'_1(v_2))) &= W_{T'}(E'_1(u), V \setminus (E'_1(u) \cup E'_1(v_2))),
\end{aligned}$$

and

$$W_T(E'_1(u), E'_1(v_2)) > W_{T'}(E'_1(u), E'_1(v_2)).$$

The only inequality holds because as we pass from T to T', the distance between a vertex of $E'_1(u)$ and a vertex of $E'_1(v_2)$ is decreased by 1. Since

$$\begin{aligned}
W(T) &= W_T(V \setminus E'_1(u)) + W_T(E'_1(u)) \\
&\quad +W_T(E'_1(u), V \setminus (E'_1(v_2) \cup E'_1(u))) + W_T(E'_1(u), E'_1(v_2))
\end{aligned}$$

and

$$W(T') = W_{T'}(V \setminus (E'_1(u))) + W_{T'}(E'_1(u))$$

$$+W_{T'}(E_1'(u), V \setminus (E_1'(v_2) \cup E_1'(u))) + W_{T'}(E_1'(u), E_1'(v_2)),$$

we have

$$W(T) - W(T') = W_T(E_1'(u), E_1'(v_2)) - W_{T'}(E_1'(u), E_1'(v_2)) > 0,$$

and thus $W(T') < W(T)$, a contradiction. So there is no pendant edge at any vertex in $e_2 \setminus \{v_1, v_2\}$. Then $T \cong D_{n,k,a}$ with $1 \leq a \leq \lfloor \frac{n-k}{2(k-1)} \rfloor$ for $k \geq 3$. Obviously, this is also true for $k = 2$. By Lemma 5.1, we have $T \cong D_{n,k,1}$. ■

For $\frac{n-1}{k-1} = 4$, let T be a k-uniform hypertree on n vertices nonisomorphic to $S_{n,k}, D_{n,k,1}$. If $k = 2$, then $T = P_{n,2}$. If $k \geq 3$, then $T \cong F_{n,k}, P_{n,k}$, and thus $W(T) \geq W(F_{n,k})$ with equality if and only if $T \cong F_{n,k}$ because we have by Theorem 4.1 that $W(F_{n,k}) < W(P_{n,k})$.

Theorem 5.3. *For $\frac{n-1}{k-1} \geq 5$, let T be a k-uniform hypertree on n vertices. Suppose that $T \not\cong S_{n,k}, D_{n,k,1}$. Then $W(T) \geq W(D_{n,k,2})$ with equality if and only if $T \cong D_{n,k,2}$.*

Proof. Let T be a k-uniform hypertree on n vertices nonisomorphic to $S_{n,k}$, $D_{n,k,1}$ with minimum Wiener index.

Let d be the diameter of T. Since $T \not\cong S_{n,k}$, we have $d \geq 3$. By similar argument as in the proof of Theorem 5.1, we have $d \leq 4$.

In the following we will show that $d = 3$. Suppose that $d = 4$.

Suppose that $k = 2$. Let $P = v_0v_1v_2v_3v_4$ be a diametral path of T. Suppose without loss of generality that $d_T(v_1) \geq d_T(v_3)$. By identifying v_2 and v_3 into v_2 and attaching a new pendant vertex v_3 at v_2, we get a tree T'. Obviously, $T' \not\cong S_{n,2}$. Suppose first that $T' \cong D_{n,2,1}$. Then T is the graph obtained from $v_0v_1v_2v_3v_4$ by attaching $n-5$ pendant vertices at v_2. By direct calculation, $W(T) > W(D_{n,2,2})$, a contradiction. Next suppose that $T' \not\cong D_{n,2,1}$. Let T_1 and T_2 be the components of $T - v_2v_3$ containing v_2 and v_3, respectively. Let $V_1 = V(T_1)$ and $V_2 = V(T_2) \setminus \{v_3\}$. Obviously, $|V_1| \geq 3$. Then

$$\begin{aligned} W(T) - W(T') &= W_T(V_2, \{v_3\}) - W_{T'}(V_2, \{v_3\}) + W_T(V_2, V_1) - W_{T'}(V_2, V_1) \\ &= -|V_2| + |V_2||V_1| > 0\,, \end{aligned}$$

and thus $W(T') < W(T)$, also a contradiction. Thus, in any case, $d = 3$, implying that $T \cong D_{n,2,a}$ with $1 \leq a \leq \lfloor \frac{n-2}{2} \rfloor$. Since $T \not\cong S_{n,2}, D_{n,2,1}$, we have by Lemma 5.1 that $T \cong D_{n,2,2}$.

Suppose that $k \geq 3$. Let $P = (v_0, e_1, v_1, e_2, v_2, e_3, v_3, e_4, v_4)$ be a diametral path of T. Suppose that there is at least one pendant edge at a vertex $u \in e_2 \setminus \{v_1, v_2\}$. For

$w \in \{u, v_1\}$, let $E(w)$ be the set of edges containing w except e_2, $E_1(w)$ be the set of vertices in those edges in $E(w)$, and $E_1'(w) = E_1(w) \setminus \{w\}$. By moving each edge in $E(u)$ from u to v_1 in T, we get a k-uniform hypertree T''. Obviously, $T'' \ncong S_{n,k}, D_{n,k,1}$. Note that

$$\begin{aligned} W_T(V \setminus E_1'(u)) &= W_{T''}(V \setminus E_1'(u)), \\ W_T(E_1'(u)) &= W_{T''}(E_1'(u)), \\ W_T(E_1'(u), V \setminus (E_1'(v_1) \cup E_1'(u))) &= W_{T''}(E_1'(u), V \setminus (E_1'(v_1) \cup E_1'(u))), \end{aligned}$$

and

$$W_T(E_1'(u), E_1'(v_1)) > W_{T''}(E_1'(u), E_1'(v_1)).$$

The only inequality holds because as we pass from T to T'', the distance between a vertex of $E_1'(u)$ and a vertex of $E_1'(v_1)$ is decreased by 1. Since

$$\begin{aligned} W(T) &= W_T(V \setminus E_1'(u)) + W_T(E_1'(u)) \\ &\quad + W_T(E_1'(u), V \setminus (E_1'(v_1) \cup E_1'(u))) + W_T(E_1'(u), E_1'(v_1)) \end{aligned}$$

and

$$\begin{aligned} W(T'') &= W_{T''}(V \setminus (E_1'(u))) + W_{T''}(E_1'(u)) \\ &\quad + W_{T''}(E_1'(u), V \setminus (E_1'(v_1) \cup E_1'(u))) + W_{T''}(E_1'(u), E_1'(v_1)), \end{aligned}$$

we have

$$W(T) - W(T'') = W_T(E_1'(u), E_1'(v_1)) - W_{T''}(E_1'(u), E_1'(v_1)) > 0,$$

and thus $W(T'') < W(T)$, a contradiction. So there is no pendant edge at any vertex in $e_2 \setminus \{v_1, v_2\}$. By similar argument as above, there is no pendant edge at any vertex in $e_3 \setminus \{v_2, v_3\}$.

Let $E(v_3)$ be the set of edges containing v_3 except e_3, $E_1(v_3)$ be the set of vertices in the edges of $E(v_3)$ and $E_1'(v_3) = E_1(v_3) \setminus \{v_3\}$. Now by moving each edge in $E(v_3)$ from v_3 to a vertex in $e_2 \setminus \{v_1, v_2\}$ of T, we get a k-uniform hypertree T^*. Obviously, $T^* \ncong S_{n,k}, D_{n,k,1}$. Let $E(v_1)$ be the set of edges containing v_1 except e_2, $E_1(v_1)$ be the set of vertices in the edges of $E(v_1)$, and $E_1'(v_1) = E_1(v_1) \setminus \{v_1\}$. Note that

$$\begin{aligned} W_T(E_1'(v_3)) &= W_{T^*}(E_1'(v_3)), \\ W_T(V \setminus E_1'(v_3)) &= W_{T^*}(V \setminus E_1'(v_3)), \end{aligned}$$

$$W_T(E_1'(v_3), V \setminus (E_1'(v_1) \cup E_1'(v_3))) \;=\; W_{T^*}(E_1'(v_3), V \setminus (E_1'(v_1) \cup E_1'(v_3))),$$

and

$$W_T(E_1'(v_3), E_1'(v_1)) > W_{T^*}(E_1'(v_3), E_1'(v_1)).$$

The only inequality holds because as we pass from T to T^*, the distance between a vertex of $E_1'(v_3)$ and a vertex of $E_1'(v_1)$ is decreased by 1. Since

$$\begin{aligned} W(T) &= W_T(E_1'(v_3)) + W_T(V \setminus E_1'(v_3)) \\ &\quad + W_T(E_1'(v_3), V \setminus (E_1'(v_1) \cup E_1'(v_3))) + W_T(E_1'(v_3), E_1'(v_1)) \end{aligned}$$

and

$$\begin{aligned} W(T^*) &= W_{T^*}(E_1'(v_3)) + W_{T^*}(V \setminus E_1'(v_3)) \\ &\quad + W_{T^*}(E_1'(v_3), V \setminus (E_1'(v_1) \cup E_1'(v_3))) + W_{T^*}(E_1'(v_3), E_1'(v_1)), \end{aligned}$$

we have

$$W(T) - W(T^*) = W_T(E_1'(v_3), E_1'(v_1)) - W_{T^*}(E_1'(v_3), E_1'(v_1)) > 0,$$

and thus $W(T^*) < W(T)$, a contradiction. Thus $d = 3$.

By similar argument as above, we may show that there is no pendant edge at any vertex in $e_2 \setminus \{v_1, v_2\}$. Then $T \cong D_{n,k,a}$ with $1 \leq a \leq \left\lfloor \frac{n-k}{2(k-1)} \right\rfloor$. Since $T \ncong S_{n,k}, D_{n,k,1}$, we have by Lemma 5.1 that $T \cong D_{n,k,2}$. ■

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