Research Article

A New Method to Find the Wiener Index of Hypergraphs

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The Wiener index is defined as the summation of distances between all pairs of vertices in a graph or in a hypergraph. Both models—graph-theoretical and hypergraph-theoretical—are used in mathematical chemistry for quantitatively studying physical and chemical properties of classical and nonclassical organic compounds. In this paper, we consider relationships between hypertrees and trees and hypercycles and cycles with respect to their Wiener indices.

1. Introduction

Let G be a simple connected graph with vertex set $V(G)$ and edge set $E(G)$. For $u, v \in V(G)$, let $d_G(u, v)$ be the distance between the vertices u and v in G , and let $W_G(u) = \sum_{v \in V(G)} d_G(u, v)$ be the sum of distances between u and all other vertices of G . The Wiener index of G is defined as follows [1]:

$$W(G) = \sum_{u, v \in V(G)} d_G(u, v) = \frac{1}{2} \sum_{u \in V(G)} W_G(u). \quad (1)$$

Let H be a connected hypergraph with vertex set $V(H)$ and edge set $E(H)$, where $V(H)$ is nonempty and each edge $e \in E(H)$ is a nonempty subset of $V(H)$. If each edge contains exactly k vertices, where $k \geq 2$, then a hypergraph H is called k -uniform. It is obvious that a 2-uniform hypergraph H corresponds to an ordinary graph. The degree $d_H(v)$ of a vertex $v \in V(H)$ is the number of edges of H which contains the vertex v . The order of H is the cardinality of its vertex set $V(H)$.

For $u, v \in V(H)$, a path from u to v in H is defined to be a sequence of distinct vertices and edges $(v_0, e_1, v_1, \dots, v_{p-1}, e_p, v_p)$ such that $v_{i-1}, v_i \in e_i$ for any $i = 1, \dots, p$, where $v_0 = u$ and $v_p = v$. For any $u, v \in V(H)$, if there exists a path from u to v , then H is connected. A k -uniform hypergraph H with $V(H) = \{v_1, \dots, v_n\}$ and

$E(H) = \{e_1, \dots, e_m\}$, where $e_i = \{v_{(i-1)(k-1)+1}, \dots, v_{(i-1)(k-1)+k}\}$, $i = 1, \dots, m$, is called a k -uniform loose path and denoted by $P_{n,k}$. A hypercycle $\mathcal{C}_p$ of length p in H is a sequence $(v_0, e_1, v_1, \dots, v_{p-1}, e_p, v_p)$, $p \geq 2$, of distinct vertices (with the sole exception that $v_0 \equiv v_p$) and distinct edges such that $v_{i-1}, v_i \in e_i$, $i = 1, \dots, p$. A hypertree is a connected hypergraph with no hypercycles. A k -uniform hypertree with m edges has exactly $1 + (k-1)m$ vertices. For a k -uniform hypertree H of order n , if there is a disjoint partition $V(H) = \{u\} \cup V_1 \cup \dots \cup V_m$ of the vertex set $V(H)$ such that $|V_1| = \dots = |V_m| = k-1$, and $E(H) = \{\{u\} \cup V_i : 1 \leq i \leq m\}$, then H is called a k -uniform hyperstar centered at u and 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.

Let H be a k -uniform hypergraph with vertex set $V(H) = \{v_1, \dots, v_n\}$. For $u, v \in V(H)$, the distance between u and v in H is denoted by $d_H(u, v)$. The Wiener index $W(H)$ is defined as the summation of distances among all unordered pairs of distinct vertices u, v in H :

$$W(H) = \sum_{\{u, v\} \subseteq V(H)} d_H(u, v). \quad (2)$$

Especially, the summation of distances from the vertex u to any other vertex is denoted by $W_H(u) = \sum_{v \in V(H)} d_H(u, v)$. Obviously, we have $W(H) = (1/2) \sum_{u \in V(H)} W_H(u)$.

Hypergraph theory has found applications in chemistry [2–7], showing a higher accuracy of molecular structure, that is, the higher accuracy of the model and the greater diversity of the behavior of its invariants. As an important descriptor of molecular structures, the Wiener index of a graph has many applications as well [8–13].

In this paper, we show relationships between Wiener indices for hypertrees and trees and for hypercycles and cycles with respect to some transformations. Let $\mathcal{T}$ be a k -uniform hypertree with at most two vertices whose

degrees are not less than 2 in each edge of $\mathcal{T}$. The following formulas are proved for a k -uniform hypertree $\mathcal{T}$ and a tree T of order n obtained from $\mathcal{T}$ by transformations:

$$W(\mathcal{T}) = (k-1)^2 W(T) - (n-1) \binom{k-1}{2}, \quad (3)$$

and for a k -uniform hypercycle $\mathcal{C}_n$ and a cycle C_n obtained from $\mathcal{C}$ by transformations:

$$W(\mathcal{C}_n) = \begin{cases} (k-1)^2 W(C_n) + n^2 \binom{k-1}{2}, & \text{if } n \text{ is odd,} \\ (k-1)^2 W(C_n) + n^2 \binom{k-1}{2} - \frac{n}{2}(k-2), & \text{if } n \text{ is even.} \end{cases} \quad (4)$$

2. Hypertrees and Trees

To prove (3), we need additional definitions and notations.

Let $\mathcal{T}$ be a k -uniform hypertree with at most two vertices whose degrees are not less than 2 in each edge of $\mathcal{T}$. Any two edges of $\mathcal{T}$ have at most one common vertex which is called a *joint vertex*; otherwise, it is called a nonjoint vertex.

We get a tree T from the hypertree $\mathcal{T}$ as follows: (1) in $\mathcal{T}$, we pick a nonjoint vertex in each pendent edge and pick all joint vertices to form vertex set $V(T)$; (2) if two vertices of $V(T)$ are in the same edge of the hypertree $\mathcal{T}$, then we connect them with an edge in T . A 4-uniform hypertree $\mathcal{T}$ and its corresponding tree T are shown in Figure 1.

The following notation is used in the rest of the paper. In k -uniform hypertree, the joint vertex is denoted by b_j , $j \geq 1$. The nonjoint vertex of each pendent edge e_i in a hypertree is denoted by a_i . The nonjoint vertex in the nonpendent edge is denoted by c_i . Figure 2 illustrates the notation above. If e is a pendent edge, we use $V(\mathcal{T}) \setminus v(e) \setminus \{b\}$ to denote delete all vertices in edge e except joint vertex b from $V(\mathcal{T})$.

Since there are $k-1$ nonjoint vertices in each pendent edge and $k-2$ nonjoint vertices in a nonpendent edge, the number of vertices in the induced tree T is n . The following equations hold for a hypertree $\mathcal{T}$ and induced tree T :

$$\begin{aligned} |E(\mathcal{T})| &= |E(T)| = n-1, \\ W_{\mathcal{T}}(a_i) &= (k-1)W_T(a_i), \end{aligned} \quad (5)$$

$$\begin{aligned} W_{\mathcal{T}}(b_i) &= (k-1)W_T(b_i), \\ 2W(\mathcal{T}) &= (k-1)^2 \sum_{a_i \in T} W_T(a_i) + (k-1) \sum_{b_i \in T} W_T(b_i) \\ &\quad + (k-2) \sum_{c_i \in \mathcal{T}} W_{\mathcal{T}}(c_i). \end{aligned} \quad (6)$$

Lemma 1. Let $\mathcal{T}$ be a hypertree with joint vertices b_i and nonjoint vertices c_i in each nonpendent edge e_i , $i = 1, \dots, s$. Then, the following equation holds:

$$\begin{aligned} \sum_{b_i \in V(\mathcal{T})} W_{\mathcal{T}}(b_i) - \sum_{c_i \in V(\mathcal{T})} W_{\mathcal{T}}(c_i) &= |E(\mathcal{T})|(k-1) \\ &= (n-1)(k-1). \end{aligned} \quad (7)$$

Proof. By induction on the number of edges, let $|E(\mathcal{T})| = 3$; then, either $\mathcal{T}$ is a k -uniform hyperstar $S_{|V(\mathcal{T})|,k}$ centered at vertex b or $\mathcal{T}$ is a k -uniform loose path of length 3.

If $\mathcal{T}$ is a k -uniform hyperstar $S_{|V(\mathcal{T})|,k}$ centered at vertex b , then there are no nonjoint vertices $c_i \in V(\mathcal{T})$, and hence we have

$$\sum_{b_i \in V(\mathcal{T})} W_{\mathcal{T}}(b_i) - \sum_{c_i \in V(\mathcal{T})} W_{\mathcal{T}}(c_i) = W_{\mathcal{T}}(b) = 3(k-1). \quad (8)$$

If $\mathcal{T}$ is a k -uniform loose path of length 3, then $\mathcal{T}$ has two joint vertices b_1 and b_2 . Choosing one nonjoint vertex $c_2 \in e_2$, by (5), we have

$$\begin{aligned} W_{\mathcal{T}}(b_1) + W_{\mathcal{T}}(b_2) - W_{\mathcal{T}}(c_2) &= 4(k-1) + 4(k-1) \\ &\quad - 5(k-1) = 3(k-1). \end{aligned} \quad (9)$$

Let $|E(\mathcal{T})| > 3$, then we choose any pendent edge $e \in E(\mathcal{T})$ connecting to joint vertex b , and consider $\mathcal{T}' = (V(\mathcal{T}) \setminus v(e) \setminus \{b\}, E(\mathcal{T}) \setminus e)$. We also choose one nonjoint vertex c_i ($i = 1, 2, \dots, r$) from nonpendent edge on the left of b . It can be seen that there is a joint vertex b_i for each c_i in the same edge. Then, it has the similar case for the right side of b (see Figure 3).

FIGURE 1: The 4-uniform hypertree $\mathcal{T}$ and the induced tree T . FIGURE 2: The k -uniform hypertree $\mathcal{T}$ and the induced tree T . FIGURE 3: A k -uniform hypertrees $\mathcal{T}$.

Since the vertices c_i and b_i belong to the same edge in $\mathcal{T}$ and $\mathcal{T}'$, they have the same increasing quality $\Delta(i)$ for their Wiener indices such that $W_{\mathcal{T}}(b_i) = W_{\mathcal{T}'}(b_i) + \Delta(i)$ and

$W_{\mathcal{T}}(c_i) = W_{\mathcal{T}'}(c_i) + \Delta(i)$. By the inductive hypothesis, we have

$$\sum_{b_i \in V(\mathcal{T}')} W_{\mathcal{T}'}(b_i) - \sum_{c_i \in V(\mathcal{T}')} W_{\mathcal{T}'}(c_i) = |E(\mathcal{T}')|(k-1) = (|E(\mathcal{T})| - 1)(k-1). \quad (10)$$

Thus, we obtain

$$\begin{aligned}
& \sum_{b_i \in V(\mathcal{T})} W_{\mathcal{T}}(b_i) - \sum_{c_i \in V(\mathcal{T})} W_{\mathcal{T}}(c_i) \\
&= \sum_{b_i \in V(\mathcal{T}), b_i \neq b} W_{\mathcal{T}}(b_i) + W_{\mathcal{T}}(b) - \sum_{c_i \in V(\mathcal{T})} W_{\mathcal{T}}(c_i) \\
&= \sum_{b_i \in V(\mathcal{T}'), b_i \neq b} W_{\mathcal{T}'}(b_i) + \sum_{b_i \in V(\mathcal{T}'), b_i \neq b} \Delta(i) + (W_{\mathcal{T}'}(b) + k - 1) - \sum_{c_i \in V(\mathcal{T}')} W_{\mathcal{T}'}(c_i) - \sum_{c_i \in V(\mathcal{T}')} \Delta(i) \\
&= \sum_{b_i \in V(\mathcal{T}')} W_{\mathcal{T}'}(b_i) - \sum_{c_i \in V(\mathcal{T}')} W_{\mathcal{T}'}(c_i) + k - 1 \\
&= (|E(\mathcal{T})| - 1)(k - 1) + k - 1 \\
&= |E(\mathcal{T})|(k - 1) \\
&= |E(T)|(k - 1) \\
&= (n - 1)(k - 1).
\end{aligned} \tag{11}$$

Theorem 1. Let T be an n -vertex tree obtained from the hypertree $\mathcal{T}$. Then,

$$W(\mathcal{T}) = (k - 1)^2 W(T) - (n - 1) \binom{k - 1}{2}. \tag{12}$$

Proof. By the definition of the Wiener index of a hypergraph, we have $\square$

$$\begin{aligned}
2W(\mathcal{T}) &= (k - 1)^2 \sum_{a_i \in V(T)} W_T(a_i) + (k - 1) \sum_{b_i \in V(T)} W_T(b_i) + (k - 2) \sum_{c_i \in V(\mathcal{T})} W_{\mathcal{T}}(c_i) \\
&= (k - 1)^2 \left[\sum_{a_i \in V(T)} W_T(a_i) + \sum_{b_i \in V(T)} W_T(b_i) \right] - (k - 1)(k - 2) \sum_{b_i \in V(T)} W_T(b_i) + (k - 2) \sum_{c_i \in V(\mathcal{T})} W_{\mathcal{T}}(c_i) \\
&= 2(k - 1)^2 W(T) - (k - 1)(k - 2) \sum_{b_i \in V(T)} W_T(b_i) + (k - 2) \sum_{c_i \in V(\mathcal{T})} W_{\mathcal{T}}(c_i) \\
&= 2(k - 1)^2 W(T) - (k - 2) \left[\sum_{b_i \in V(\mathcal{T})} W_{\mathcal{T}}(b_i) - \sum_{c_i \in V(\mathcal{T})} W_{\mathcal{T}}(c_i) \right].
\end{aligned} \tag{13}$$

Then,

$$\begin{aligned}
W(\mathcal{T}) &= (k - 1)^2 W(T) - \frac{k - 2}{2} \\
&\quad \cdot \left[\sum_{b_i \in V(\mathcal{T})} W_{\mathcal{T}}(b_i) - \sum_{c_i \in V(\mathcal{T})} W_{\mathcal{T}}(c_i) \right].
\end{aligned} \tag{14}$$

By Lemma 1, we get

$$W(\mathcal{T}) = (k - 1)^2 W(T) - (n - 1) \binom{k - 1}{2}. \tag{15}$$

$\square$

Corollary 1. Let $S_{t,k}$ be a k -uniform hyperstar of order t . Then,

$$W(S_{t,k}) = (t - 1)^2 - \frac{(t - 1)(k - 2)}{2}. \tag{16}$$

Proof. By $W(S_{((t-1)/(k-1))+1}) = ((t-1)/(k-1))^2$ and from Theorem 1, we have

$$\begin{aligned}
W(S_{t,k}) &= (k - 1)^2 W(S_{((t-1)/(k-1))+1}) - \left(\frac{t-1}{k-1} + 1 - 1 \right) \binom{k-1}{2} \\
&= (k - 1)^2 \left(\frac{t-1}{k-1} \right)^2 - \left(\frac{t-1}{k-1} \right) \binom{k-1}{2} \\
&= (t - 1)^2 - \frac{(t - 1)(k - 2)}{2}.
\end{aligned} \tag{17}$$

$\square$

Corollary 2. Let $P_{t,k}$ be a k -uniform loose path of order t . Then,

$$W(P_{t,k}) = (k-1)^2 \binom{((t-1)/(k-1)) + 2}{3} - \frac{(t-1)(k-2)}{2}. \quad (18)$$

Proof. It follows from Theorem 1 and by $W(P_n) = \binom{n+1}{3}$. $\square$

3. Hypercycles and Cycles

Let us consider the hypercycle $\mathcal{C}_n$ with n joint vertices b_i , $i = 1, \dots, n$. If b_i and b_j , $i \neq j$, are in the same edge in $\mathcal{C}_n$, then we connect them with an edge and get an n -vertex cycle C_n from the hypercycle $\mathcal{C}_n$. We denote by a_i a nonjoint vertex in each edge e_i , $i = 1, \dots, n$. The following statement gives us the relationship between Wiener indices of $\mathcal{C}_n$ and C_n .

TABLE 1: The Wiener index of k -uniform hypercycles and corresponding cycles.

$W(\mathcal{C}_2) = (k-1)^2 + 4 \binom{k-1}{2} - (k-2)$	$W(C_2) = 1$
$W(\mathcal{C}_3) = 3(k-1)^2 + 9 \binom{k-1}{2}$	$W(C_3) = 3$
$W(\mathcal{C}_4) = 8(k-1)^2 + 16 \binom{k-1}{2} - 2(k-2)$	$W(C_4) = 8$
$W(\mathcal{C}_5) = 15(k-1)^2 + 25 \binom{k-1}{2}$	$W(C_5) = 15$
$W(\mathcal{C}_6) = 27(k-1)^2 + 36 \binom{k-1}{2} - 3(k-2)$	$W(C_6) = 27$
$W(\mathcal{C}_7) = 42(k-1)^2 + 49 \binom{k-1}{2}$	$W(C_7) = 42$

Theorem 2.

$$W(\mathcal{C}_n) = \begin{cases} (k-1)^2 W(C_n) + n^2 \binom{k-1}{2}, & \text{if } n \text{ is odd,} \\ (k-1)^2 W(C_n) + n^2 \binom{k-1}{2} - \frac{n}{2}(k-2), & \text{if } n \text{ is even.} \end{cases} \quad (19)$$

Proof. If n is odd, the following equations are obtained by the definition of Wiener index:

$$2W(C_n) = n \left(1 + 1 + 2 + 2 + \dots + \frac{n-1}{2} + \frac{n-1}{2} \right) = \frac{n^3 - n}{4},$$

$$W_{\mathcal{C}_n}(b_i) = \frac{(n^2 + 2n + 1)(k-1)}{4} - \frac{n+1}{2},$$

$$W_{\mathcal{C}_n}(a_i) = \frac{(n^2 + 4n - 1)(k-1)}{4} - \frac{n+1}{2},$$

$$\begin{aligned} W(\mathcal{C}_n) &= \frac{1}{2} n W(b_i) + \frac{1}{2} n (k-2) W(a_i) \\ &= \frac{k-1}{2} \frac{n^3 - n}{4} + \frac{n(n^2 + 4n - 1)}{4} \frac{(k-1)(k-2)}{2} \\ &= \frac{k-1}{2} \frac{n^3 - n}{4} + \left(\frac{n^3 - n}{8} + \frac{n^2}{2} \right) (k-1)(k-2) \\ &= (k-1) W(C_n) + \left(W(C_n) + \frac{n^2}{2} \right) (k-1)(k-2) \\ &= (k-1)^2 W(C_n) + n^2 \binom{k-1}{2}. \end{aligned} \quad (20)$$

If n is even, then by (5) and (6) we have the following equations:

$$2W(C_n) = n \left(1 + 1 + 2 + 2 + \dots + \frac{n-2}{2} + \frac{n-2}{2} + \frac{n}{2} \right) = \frac{n^3}{4},$$

$$W_{\mathcal{C}_n}(b_i) = \frac{(n^2 + 2n)(k-1)}{4} - \frac{n}{2},$$

$$W_{\mathcal{C}_n}(a_i) = \frac{(n^2 + 4n)(k-1)}{4} - \frac{n+2}{2},$$

$$\begin{aligned} W(\mathcal{C}_n) &= \frac{1}{2} n W(b_i) + \frac{1}{2} n (k-2) W(a_i) \\ &= \frac{k-1}{2} \frac{n^3}{4} + \frac{(n^3 + 4n^2)}{4} \frac{(k-1)(k-2)}{2} + \frac{n}{2} \\ &= \frac{k-1}{2} (2W(C_n) - n) + (2W(C_n) + n^2) \\ &\quad \cdot \frac{(k-1)(k-2)}{2} + \frac{n}{2} \\ &= (k-1)^2 W(C_n) + n^2 \binom{k-1}{2} - \frac{n}{2}(k-2). \end{aligned} \quad (21)$$

Table 1 presents the Wiener index for the k -uniform hypercycles $\mathcal{C}_i$ and their corresponding cycles C_i , $2 \leq i \leq 7$. $\square$

Data Availability

No data were used to support this study.

Conflicts of Interest

The authors Yalan Li and Bo Deng declare that there are no conflicts of interest regarding the publication of this paper.

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