



# Article Wiener index of uniform hypergraphs induced by trees

## Andrey Alekseevich Dobrynin<sup>1,\*</sup>

- <sup>1</sup> Sobolev Institute of Mathematics, Siberian Branch of the Russian Academy of Sciences, Novosibirsk, 630090, Russia.
- \* Correspondence: dobr@math.nsc.ru

Received: 5 September 2019; Accepted: 23 October 2019; Published: 2 November 2019

**Abstract:** The Wiener index W(G) of a graph *G* is defined as the sum of distances between its vertices. A tree *T* generates *r*-uniform hypergraph  $H_{r,k}(T)$  by the following way: hyperedges of cardinality *r* correspond to edges of the tree and adjacent hyperedges have *k* vertices in common. A relation between quantities W(T) and  $W(H_{r,k}(T))$  is established.

Keywords: Tree, hypergraph, Wiener index.

MSC: 05C12

## 1. Introduction

**I** n this paper we are concerned with undirected connected graphs *G* with vertex set *V*(*G*) and edge set E(G). The degree of a vertex is the number of edges that are incident to the vertex. Degree of a vertex *v* is denoted by deg(*v*). If *u* and *v* are vertices of *G*, then the number of edges in a shortest path connecting them is said to be their distance and is denoted by  $d_G(u, v)$ . Distance of a vertex *v* is the sum of distances from *v* to all vertices of a graph,  $d_G(v) = \sum_{u \in V(G)} d(v, u)$ . The Wiener index is a graph invariant defined as the sum of distances between all vertices of *G*:

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

It was introduced as a structural descriptor for tree-like molecular graphs [1]. Details on the mathematical properties and chemical applications of the Wiener index can be found in books [2–7] and reviews [8–13]. A number of articles are devoted to comparing of the index of a graph and its derived graphs such as the line graph, the total graph, thorny and subdivision graphs of various kind (see, for example, [14–17]). Hypergraphs generalize graphs by extending the definition of an edge from a binary to an *r*-ary relation. Wiener index of some classes of hypergraphs was studied in [18–20]. Chemical applications of hypergraphs were discussed in [21,22].

Define a class of *r*-uniform hypergraphs  $H_{r,k}(T)$  induced by *n*-vertex trees *T*. Edges of a tree correspond to hyperedges of cardinality *r* and adjacent hyperedges have *k* vertices in common,  $1 \le k \le \lfloor r/2 \rfloor$ . Examples of a tree and the corresponding hypergraph are shown in Figure 1. The number of vertices of  $H_{r,k}(T)$  is equal to (n-2)(r-k) + r. We are interesting in finding a relation between quantities W(T) and  $W(H_{r,k}(T))$ .



**Figure 1.** Tree *T* and the induced hypergraph  $H_{7,2}(T)$ .

### 2. Main result

Wiener indices of a tree and its induced hypergraph satisfy the following relation.

**Theorem 1.** For the induced hypergraph  $H_{r,k}(T)$  of a tree T with n vertices,

$$W(H_{r,k}(T)) = (r-k)^2 W(T) + n\binom{k}{2} - (n-1)\binom{r-2k+1}{2}.$$

This result may be useful for ordering of Wiener indices of hypergraphs. If *r* and *k* are fixed, then the ordering of the Wiener index of induced hypergraphs  $H_{r,k}$  for *n*-vertex trees is completely defined by the ordering of the index of trees. In particular,

$$W(H_{r,k}(S_n)) \le W(H_{r,k}(T)) \le W(H_{r,k}(P_n))$$

for any *n*-vertex tree *T*, where  $S_n$  and  $P_n$  are the star and the path with *n* vertices,

$$W(H_{r,k}(S_n)) = (r(n-1)[2n(r-2k)+8k-3r-1]+k(n-2)[k(2n-3)+1])/2,$$
  
$$W(H_{r,k}(P_n)) = n(r-k)[(r-k)n^2+10k-4r-3]/6+2k^2-k(2r+1)+r(r+1)/2.$$

#### 3. Proof of Theorem 1

The edge subdivision operation for an edge  $(x, y) \in E(G)$  is the deletion of (x, y) from graph *G* and the addition of two edges (x, v) and (v, y) along with the new vertex *v*. Vertex *v* is called the subdivision vertex. Denote by  $T_e$  the tree obtained from the subdivision of edge *e* in a tree *T*. The distance  $d_G(v, U)$  from a vertex  $v \in V(G)$  to a vertex subset  $U \subseteq V(G)$  is defined as  $d_G(v, U) = \sum_{u \in U} d_G(v, u)$ .

**Lemma 2.** Let  $T_{e_1}, T_{e_2}, \ldots, T_{e_{n-1}}$  be trees obtained by subdivision of edges  $e_1, e_2, \ldots, e_{n-1}$  of *n*-vertex tree *T* with subdivision vertices  $v_1, v_2, \ldots, v_{n-1}$ , respectively. Then

$$d_{T_{e_1}}(v_1) + d_{T_{e_2}}(v_2) + \dots + d_{T_{e_{n-1}}}(v_{n-1}) = 2W(T).$$

**Proof.** Let *v* be the subdivision vertex of edge e = (x, y) of a tree *T*. Denote by  $V_x$  and  $V_y$  the sets of vertices of two connected components after deleting edge *e* from *T* where  $x \in V_x$  and  $y \in V_y$ . Since  $d_T(x) = d_T(x, V_x) + |V_y| + d_T(y, V_y)$  and  $d_T(y) = d_T(y, V_y) + |V_x| + d_T(x, V_x), d_T(x, V_x) + d_T(y, V_y) = (d_T(x) + d_T(y) - n)/2$ . Then

$$d_{T_e}(v) = \sum_{u \in V_x} [d_{T_e}(v, x) + d_T(x, u)] + \sum_{u \in V_y} [d_{T_e}(v, y) + d_T(y, u)]$$
  
=  $d_T(x, V_x) + d_T(y, V_y) + n = (d_T(x) + d_T(y) + n)/2.$ 

Klein *et al.* [23] proved that  $\sum_{v \in V(T)} \deg(v) d_T(v) = 4W(T) - n(n-1)$  for an arbitrary *n*-vertex tree *T*. Then

$$2\sum_{i=1}^{n-1} d_{T_{e_i}}(v_i) = \sum_{(x,y)\in E(T)} (d_T(x) + d_T(y) + n)$$
  
= 
$$\sum_{v\in V(T)} \deg(v)d_T(v) + n(n-1) = 4W(T).$$

For convenience, we assume that pendent hyperedges are also adjacent with fictitious hyperedges shown by dashed lines in Figure 2. Denote by  $B_i$ , i = 1, 2, ..., n, the vertices of a hypergraph  $H = H_{r,k}(T)$  belonging to hyperedge intersections and let  $A = V(H) \setminus B_1 \cup B_2 \cup \cdots \cup B_n$ . We assume that edge  $E_i$  of the induced



Figure 2. The hyperedges shown by dashed lines

hypergraph corresponds to edge  $e_i$  of the source tree T, i = 1, 2, ..., n - 1. Let  $d_G(U) = \sum_{u \in U} d_G(u)$  for  $U \subseteq V(G)$ . Then the Wiener index of H can be represented as follows:

$$W(H) = \frac{1}{2} \left( \sum_{i=1}^{n-1} d_H(E_i \cap A) + \sum_{i=1}^n d_H(B_i) \right).$$
(1)

Let  $u \in E_i \cap A$  and  $v_i$  be the subdivision vertex of edge  $e_i$  in T, i = 1, 2, ..., n - 1. Then

$$\begin{array}{lll} d_{H}(u) &=& (r-2k-1)+k+k+2(r-k)+\dots+2(r-k)+3(r-k)+\dots+3(r-k)+\dots\\ &=& (r-2k-1)-2(r-2k)+(r-k)+(r-k)+2(r-k)+\dots+2(r-k)\\ && +3(r-k)+\dots+3(r-k)+4(r-k)+\dots+4(r-k)+\dots\\ &=& (r-k)d_{T_{e_{i}}}(v_{i})-2(r-2k)+(r-2k-1). \end{array}$$

Summing this equality for all vertices of intersection  $E_i \cap A$ , we have  $d_H(E_i \cap A) = (r - 2k)d_H(u) = (r - 2k)[(r - k)d_{T_{e_i}}(v_i) - (r - 2k + 1)]$ . Applying Lemma 2, we can write

$$\sum_{i=1}^{n-1} d_H(E_i \cap A) = (r-2k) \left( (r-k) \sum_{i=1}^{n-1} d_{T_{e_i}}(v_i) - (n-1)(r-2k+1) \right)$$
  
=  $(r-2k) \left[ 2(r-k)W(T) - (n-1)(r-2k+1) \right].$  (2)

Let  $u \in B_i$  and vertex  $v_i$  of T corresponds to this hyperedge intersection, i = 1, 2, ..., n. Then

$$d_H(u) = (k-1) + (r-k) + \dots + (r-k) + 2(r-k) + \dots + 2(r-k) + 3(r-k) + \dots + 3(r-k) + \dots$$
  
=  $(r-k)d_T(v_i) + (k-1).$ 

Summing this equality for all vertices of the hyperedge intersection  $B_i$ , we have  $d_H(B_i) = kd_H(u) = k[(r-k)d_T(v_i) + (k-1)]$ . For vertices of all intersections,

$$\sum_{i=1}^{n} d_H(B_i) = k \left[ (r-k) \sum_{i=1}^{n} d_T(v_i) + n(k-1) \right] = 2k(r-k)W(T) + nk(k-1).$$
(3)

Substitution expressions (2) and (3) back into Equation (1) completes the proof.

Acknowledgments: This work is supported by the Russian Foundation for Basic Research (project numbers 19–01–00682 and 17–51–560008).

Conflicts of Interest: "The author declare no conflict of interest."

#### References

- [1] Wiener, H. (1947). Structural determination of paraffin boiling points. *Journal of the American Chemical Society*, 69(1), 17-20.
- [2] Balaban, A. T., Motoc, I., Bonchev, D., & Mekenyan, O. (1983). Topological indices for structure-activity correlations. In *Steric effects in drug design* (pp. 21-55). Springer, Berlin, Heidelberg.
- [3] Gutman, I., & Furtula, B. (Eds.) (2012). *Distance in Molecular Graphs Theory*. Mathematical chemistry monographs, 12, Univ. Kragujevac, Kragujevac, Serbia.

- [4] Gutman, I., & Furtula, B. (Eds.) (2012). Distance in Molecular Graphs Applications. Mathematical chemistry monographs, 13, Univ. Kragujevac, Kragujevac, Serbia.
- [5] Gutman, I., & Polansky, O. E. (1986). Mathematical Concepts in Organic Chemistry, Springer-Verlag, Berlin.
- [6] Todeschini, R., & Consonni, V. (2008). Handbook of molecular descriptors (Vol. 11). John Wiley & Sons.
- [7] Trinajstić, N. (1992). Chemical Graph Theory. CRC Press, Boca Raton.
- [8] Dobrynin, A. A., Entringer, R., & Gutman, I. (2001). Wiener index of trees: theory and applications. Acta Applicandae Mathematica, 66(3), 211-249.
- [9] Dobrynin, A. A., Gutman, I., Klavžar, S., & Žigert, P. (2002). Wiener index of hexagonal systems. *Acta Applicandae Mathematica*, 72(3), 247-294.
- [10] Nikolić, S., & Trinajstić, N. (1995). The Wiener index: Development and applications. *Croatica Chemica Acta*, 68(1), 105-129.
- [11] Entringer, R. C., Jackson, D. E., & Snyder, D. A. (1976). Distance in graphs. Czechoslovak Mathematical Journal, 26(2), 283-296.
- [12] Knor, M., Škrekovski, R., & Tepeh, A. (2015). Mathematical aspects of Wiener index. Ars Mathematica Contemporanea, 11(2), 327–352.
- [13] Entringer, R. C. (1997). Distance in graphs: trees. *Journal of Combinatorial Mathematics and Combinatorial Computing*, 24, 65–84.
- [14] Eliasi, M., Raeisi, G., & Taeri, B. (2012). Wiener index of some graph operations. *Discrete Applied Mathematics*, 160(9), 1333-1344.
- [15] Gutman, I. (1998). Distance of thorny graphs. Publications de l'Institut Mathématique (Beograd), 63(31-36), 73-74.
- [16] Knor, M., & Škrekovski, R. (2014). Wiener index of line graphs. In Quantitative Graph Theory: Mathematical Foundations and Applications, 279-301. 279–301.
- [17] Dobrynin, A. A., & Mel'nikov, L. S. (2012). Wiener index of line graphs. In: *Distance in Molecular Graphs Theory,* Gutman, I., & Furtula, B. (Eds.). Univ. Kragujevac, Kragujevac, Serbia, 85–121.
- [18] Guo, H., Zhou, B., & Lin, H. (2017). The Wiener index of uniform hypergraphs. MATCH Communications in Mathematical and in Computer Chemistry, 78, 133-152.
- [19] Rani, L. N., Rajkumari, K. J., & Roy, S. (2019). Wiener Index of Hypertree. In Applied Mathematics and Scientific Computing (pp. 497-505). Birkhäuser, Cham.
- [20] Sun, L., Wu, J., Cai, H., & Luo, Z. (2017). The Wiener index of *r*-uniform hypergraphs. Bulletin of the Malaysian Mathematical Sciences Society, 40(3), 1093-1113.
- [21] Konstantinova, E. V., & Skorobogatov, V. A. (2001). Application of hypergraph theory in chemistry. Discrete Mathematics, 235(1-3), 365-383.
- [22] Konstantinova, E. (2000). Chemical hypergraph theory. *Lecture Notes from Combinatorial & Computational Mathametics Center, http://com2mac. postech. ac. kr.*
- [23] Klein, D. J., Mihalić, Z., Plavšić, D., & Trinajstić, N. (1992). Molecular topological index: A relation with the Wiener index. Journal of Chemical Information and Computer Sciences, 32(4), 304-305.



© 2019 by the authors; licensee PSRP, Lahore, Pakistan. This article is an open access article distributed under the terms and conditions of the Creative Commons Attribution (CC-BY) license (http://creativecommons.org/licenses/by/4.0/).