New calculation of the Wiener index for some particular graphs

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Abstract
In this paper, we give new result for calculating the Wiener index for some particular graphs. As the path and therefore the distance between two vertices of a tree is unique, the Wiener index of a tree is much easier to compute than that of an arbitrary graph. In the following, we will show new formulas for computing the Wiener index, in the first part direct ones and in the second part recursive ones that require certain characteristics of the graphs but in case their requirements are satisfied may make the calculation of the Wiener index easier by far.

Keywords: Graph, Tree, Wiener Index, Distance, Root, Degree.

1 Introduction

The first investigations into the Wiener index were made by Harold Wiener in 1947 who realized that there are correlations between the boiling points of paraffin and the structure of the molecules [12]. In particular he mentions in his article that the boiling point t_B can be quite closely approximated by the formula: t_B = aw + bp + c, where W is the Wiener index, p the polarity number and a, b and c are constants for a given isomeric group. Since then it has become one of the most frequently used topological indices in chemistry, as molecules are usually modeled as undirected graphs, especially trees. For example, in the drug design process, the aim is the construction of chemical compounds with certain properties, which not only depend on the chemical formula but also strongly on the molecular structure, as one can easily see when considering cocaine and scopolamine, both having the chemical formula $C_{17}\ H_{21}\ NO_4$: Furthermore, there are many situations in communication, facility location, cryptology, architecture etc. where the Wiener index of the corresponding graph or the average distance [24, 25] is of great interest. A graph G is a triple consisting of a vertex set V (G), an edge set E(G), and a relation that associates with each edge two vertices called its end points[5]. A connected graph is a graph such that for each pair u, v (two distinct vertices, there is a path of vertices connecting these two points. A graph is simple if two vertices there is at most one edge. The distance between two vertices v_i and v_j in a graph G is the length of the shortest path (number of edge) connecting these two vertices [4, 9, 10, 20, 21], and we note d(v_i , v_j). The diameter of a plane tree A is by definition the number of edges of the longest path in this tree A[6]. The wiener index W(G) a connected graph G is the sum of all distances between pairs of vertices of G [7, 8, 17, 23]:

$$w(G) = \sum_{\{u,v\} \in V(G)} d(u,v)$$

The wiener index of a vertex v in G is defined as:

$$w(v.\ G) = \sum_{u \in V(G)} d(u,v).$$

The average behaviour of the Wiener index was first studied by Entringer et al [18], who considered so-called simply generated families of trees (introduced by Meir and Moon). They were able to prove that the average Wiener index is asymptotically Kn^5 where the constant K depends on the specific family of trees. Thus the average value of the wiener index is apart from a constant factor, the geometric mean of the extremal values, which are given for the star s_n and the path p_n respectively [13, 18];

$$(n-1)^2 = W(S_n) \le W(T) \le W(P_n) = \binom{n+1}{3}$$

for all trees T with n vertices. Dobrynin and Gutman [12] calculated numerical values for the average Wiener index of trees and chemical trees of small order by direct computer calculation. The average Wiener index of a tree has been determined, in a different context, in a paper of Moon [15]. The aim of this note is to extend the cited result to trees with restricted degree, especially chemical trees. In fact, the enumeration method for chemical trees is older than the result of otter and goes back to [5]. We consider an auxiliary value, D(T) denoting the sum of the distances of all vertices from the root. This is also known as the total height of the tree T [14]. The value D(T) can be calculated recursively from the branches $T_1, T_2, \dots, T_k$ of T, viz T [22].

$$D(T) = \sum_{i=1}^{k} D(T_i) + |T| - 1,$$

where $|T|$ is the size (number of vertices) of T. Now, we use the following recursive relation from [18], which relates the Wiener index of a rooted tree T with the Wiener indices of its branches $T_1, T_2, \dots, T_k$:

$$W(T) = D(T) + \sum_{i=1}^{k} W(T_i) + \sum_{i=j} (D(T_i) + |T|)|T_j|,$$

where the last sum goes over all k(k - 1) pairs of different branches.

2 Direct formulas

The first formula we are going to show is a very basic one and was found by H. Wiener in 1947 (see [12]). While the definition of the Wiener index puts its stress on how far one has to go from each vertex to reach all other vertices, this formula counts how often one has to pass each edge.

3 Main result

In this paper, we give new results for calculating the Wiener index for some particular graphs. In the end we give an application of its results on particular families of graphs

Definition 1 Let e = (u, v) ∈ E(T) be an edge of the tree T. The sub trees T_u and T_v are defined as the connected components of T containing u and v, respectively. The order of the sub trees is denoted by $n_u\ (e) = |V(\ T_u)|$ and $n_v\ (e) = |V(\ T_v)|$.

Theorem 2 Let T be a tree, then:

$$W(T) = \sum_{e=(u,v)\in E(T)} n_u\ (e) n_v\ (e)$$

$$= \sum_{e=(u,v)\in E(T)} |V(\ T_u)|\ |V(\ T_v)|$$

Proof As T is a tree, the unique path between a vertex $x \in\ V(\ T_u\ )$ and a vertex $y \in$ $V(\ T_v)$ must contain e. If x and y are chosen in a different way, e is not part of the path between them. Therefore $n_u\ (e)\ n_v\ (e)$ is exactly the number of times how often e belongs to a path between two vertices of T. Then the sum of $n_u\ (e)\ n_v\ (e)$ over all edges of T must be the Wiener index of T.

Remark 3 Dobrynin and Gutman give another proof of theorem 2, in a more general way in [3, 11, 19]. In addition to that they show for what types of graphs equation 2, holds and that for all other cases the right-hand side of equation 2, which is denoted as the new graph invariant W_ called Szeged index, is greater than the corresponding Wiener index. To be able to define W^* one has to generalize the definition of T_u and T_v first, which we are going to show in the following definition to give an idea of this closely related graph invariant before continuing with our original topic.

Definition 4 Let $e = (u, v) \in E(G)$ be an edge of the graph G. The sets $B_u\ (e)$ and $B_v\ (e)$ of vertices of G are defined as

$$B_u\ (e) = x \in\ V(\mathrm{G})\ :\ \ \mathrm{d(x,u)} < \mathrm{d(x,v)}$$
$$B_v\ (e) = y \in\ V(\mathrm{G})\ :\ \ \mathrm{d(y,v)} < \mathrm{d(y,u)}.$$

The cardinalities of the sets are denoted by $n_u\ (e) = |B_u\ (e)|$ and $n_v\ (e) = |B_v\ (e)|$.

Lemma 5 If the graphs G_i have the same number of vertices if $m_i = m$ for i = 1,2, … , n then:

$$\begin{cases} \mathrm{w}(\mathrm{s}, \mathrm{G}_{m_i}) = \mathrm{w}\left(\mathrm{s}, \mathrm{G}_{m_j}\right) \\ \mathrm{G}_{m_i} = \ \mathrm{G}_{m_j} = \mathrm{G_m} \qquad \text{for } \mathrm{i}, \mathrm{j} \in \{1{,}2, \dots, \mathrm{n}\} \\ \mathrm{N} = \mathrm{nm} - \mathrm{n} + 1 \end{cases}$$

Or d(u, v) = d(u, s) + d(s, v) then:

$$\sum_{u\in V^*\left(\mathrm{G}_{m_i}\right)} \sum_{v\in V^*\left(\mathrm{G}_{m_j}\right)} d(u,v)$$

$$= \left(m_j - 1\right) \sum_{u\in V^*\left(\mathrm{G}_{m_i}\right)} d(u,s) + (m_i - 1) \sum_{v\in V^*\left(\mathrm{G}_{m_j}\right)} d(s,v)$$

$$= \left(m_j - 1\right) w\left(s, \mathrm{G}_{m_i}\right) + (m_i - 1) w\left(s, \mathrm{G}_{m_j}\right)$$

$$. \quad = [W(G_i) + \left(\mathrm{D}(G_i) + |G|\right) \left|G_j\right|]$$

Theorem 6 Let G be a graph then:

$$W(G_N) = \sum_{i=1}^{k} W\left(\mathrm{G}_{m_i}\right) + \sum_{i=1}^{k-1} \sum_{j=i+1}^{k} [W(G_i) + \left(\mathrm{D}(G_i) + |G|\right) \left|G_j\right|] \,,$$

Proof

$$W(G_N) = \sum_{u\in v\,(G_N)} \sum_{v\in v\,(G_N)} d(u,v)$$

$$= \sum_{u\in V^*\left(\mathrm{G}_{m_{n-1}}\right)} \sum_{v\in V^*\left(\mathrm{G}_{m_n}\right)} d(u,v) + \sum_{u\in V^*\left(\mathrm{G}_{m_{n-2}}\right)} \sum_{v\in V^*\left(\mathrm{G}_{m_{n-1}}\right)} d(u,v) +$$

$$\sum_{u\in V^*\left(\mathrm{G}_{m_{n-2}}\right)} \sum_{v\in V^*\left(\mathrm{G}_{m_n}\right)} d(u,v) + \cdots$$

$$+ \sum_{u\in V^*\left(\mathrm{G}_{m_i}\right)} \sum_{v\in V^*\left(\mathrm{G}_{m_{i+1}}\right)} d(u,v) + \cdots +$$

$$\sum_{u\in V^*\left(\mathrm{G}_{m_i}\right)} \sum_{v\in V^*\left(\mathrm{G}_{m_n}\right)} d(u,v) + \cdots + \sum_{u\in V^*\left(\mathrm{G}_{m_1}\right)} \sum_{v\in V^*\left(\mathrm{G}_{m_2}\right)} d(u,v) + \cdots +$$

$$\sum_{u\in V^*\left(\mathrm{G}_{m_1}\right)} \sum_{v\in V^*\left(\mathrm{G}_{m_n}\right)} d(u,v)$$

$$= \sum_{i=1}^{k} W\left(\mathrm{G}_{m_i}\right) + \sum_{i=1}^{k-1} \sum_{j=i+1}^{k} \left(\sum_{u\in V^*\left(\mathrm{G}_{m_i}\right)} \sum_{v\in V^*\left(\mathrm{G}_{m_j}\right)} d(u,v) \right)$$

$$= \sum_{i=1}^{k} W\left(\mathrm{G}_{m_i}\right) + \sum_{i=1}^{k-1} \sum_{j=i+1}^{k} [W(G_i) + \left(\mathrm{D}(G_i) + |G|\right) \left|G_j\right|] \,.$$

4 Application

We will give an application in Case of a fan F_m

Let F_m be the fan (see Figure 1).

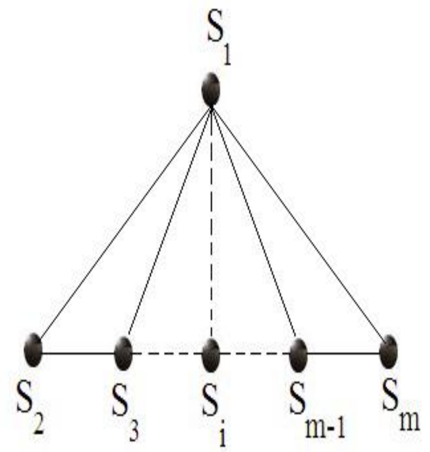

Figure 1: The fan F_m

$$W(S_i, \ F_m)\begin{cases} m-1 & \text{for } i=1 \\ 2m-4 & \text{for } i=1,\dots,m \\ 2m-3 & \text{for } i=1,\dots,m \end{cases}$$

Proposition 7 The wiener index of F_m [10] is:

$$\mathrm{W}(F_m) = m^2 - 3m + 3, \qquad m \geq 3.$$

Let G_N be the fan formed by n stars F_m connected by a vertex s.
G_N is $F_m \, . F_m \, . F_m, \dots, F_m$ (see Figure 2).

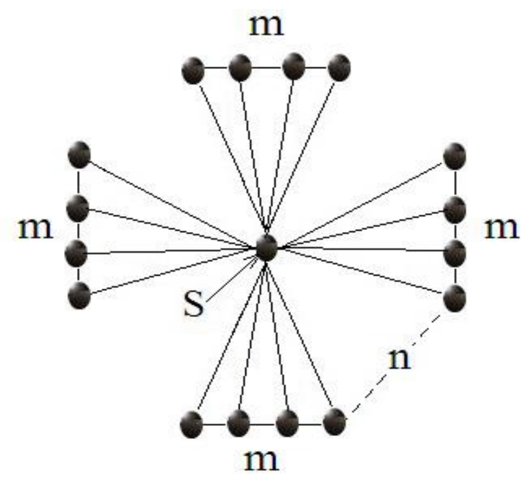

Figure 2: Fan-graphs $F_m \ . F_m, \dots, F_m$

Proposition 8 The wiener index of star graph $G_N = \ G_m, G_m, \dots, G_m$ [8]is:

$$W(G_N) = nW(G_m) + n(n-1)(m-1)w(s, G_m)$$

Theorem 9 The wiener index of Fan-graph $G_N = \ F_m \ . F_m, \dots, F_m$ is:

$$W(G_N) = n(m^2 - 3m + 3)\, n(n-1)^2\, (m-1) \qquad \text{with } n \geq 1, \ m \geq 3$$

Proof We use the Proposition 8.

$$W = (F_m \ .F_m, \dots, F_m) = nw(F_m) + n(n-1)(m-1)w((S_i, \ F_m)$$

$$= n(m^2 - 3m + 3)\, n(n-1)^2\, (m - 1)$$

Let G_N be star-fan composed by $m - 2$ Fan $F_3 \ .F_{4\,.} \ F_5, \dots, F_m$ (see Figure 3).

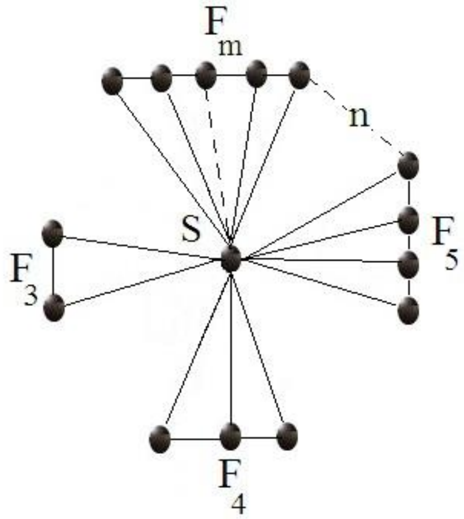

Figure 3: Fan-graph $F_3 \ .F_{4\,.} \ F_5, \dots, F_m$

Theorem 10 The wiener index of $G_N = W(F_3 \ .F_{4\,.} \ F_5, \dots, F_{m_i})$ is:

$$W(G_N) = \frac{m^4 + 6m^3 + 6m^2 + m}{4}, \qquad m \geq 3$$

Proof We use the theorem 6.

$$W(F_3 \ .F_{4\,.} \ F_5, \dots, F_m)$$

$$= \sum_{i=3}^{m} W(\mathrm{F_i}) + \sum_{i=3}^{m-1} \sum_{j=i+1}^{m} [(m_j - 1)w(s, F_{m_i}) + (m_i - 1)w\left(s, F_{m_j}\right)]$$

$$= \sum_{i=3}^{m} (i^2 - 3i + 3) + \sum_{i=3}^{m-1} \sum_{j=i+1}^{m} [(j-1)(i-1) + ij - i - j + 1]$$

$$= \sum_{i=3}^{m} (i^2 - 3) + \sum_{i=3}^{m-1} i + 3[(m-3) + 1] +$$

$$+ \sum_{i=3}^{m-1} [\sum_{j=i+1}^{m} ij - i - \sum_{j=i+1}^{m} j + \sum_{j=i+1}^{m} 1 - j]$$

$$= \sum_{i=3}^{m} (i^2 - 3) + \sum_{i=3}^{m-1} i + 3[(m-3) + 1]$$

$$+ \sum_{i=3}^{m-1} [\frac{i(m-i)(m+i+1)}{2} - i - \frac{(m-i)(m+i+1)}{2}$$

$$+ (m-i)(1-i)]$$

$$= \frac{m^4 + 6m^3 + 6m^2 + m}{4}.$$

Table : Wiener index of the product graph after each iteration

m	4	5	8	12	15
n	3	5	9	11	18
$W(G_N)$	39	385	4419	13321	76122

Table : Fan-graph $F_m \ . F_m, \dots, F_m$

5 Conclusion

In this paper, we give new results, for calculating the Wiener index for some particular graphs. In the end we give an application of its results on particular families of graphs

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6 References

[1] A. A. Dobrynin and I. Gutman," The Average Wiener Index of Trees and Chemical Trees", J. Chem. Inf. Comput. Sci., 39:679-683,(1999).

[2] A. Cayley," A theorem on trees", Quart J. Math. Oxford Ser., 23:376- 378,(1889).

[3] A. Dobrynin and I. Gutman,"On a graph invariant related to the sum of all distances in a graph", Publ. Inst. Math. (Beograd), 56, 18-22,(2010).

[4] B. Di Fabio and C. Landi,"The Edit Distance for Reeb Graphs of Sur- faces", Disc. Comp. Geom, vol. 55, no. 2, pp, 423-461,(2016).

[5] D. B. West, "Introduction to Graph Theory", Second Edition, University of Illinois - Urbana, (2002).

[6] Gabr Al Hagri (G. Al Hagri),"The Diameter of a Tree Composed", ISSN:2617-31 58 www.abhath-ye.com ,(2019).

[7] G. Al Hagri, M. El Marraki,"Calculation of The wiener index of some particular trees", Journal of Theoretical and Applied Information Technology, Vol.22 No.2,(2010).

[8] G. AL Hagri, M. Essalih and M. El Marraki,"The wiener index of some particular graph", IJCSNS International Journal of Computer Science and Network Security. VOL.11 No.5, May (2011).

[9] G . Indulal,"Distance Spectrum of Graph Compositions", ARS Mathematic Contemporaneity 2, 93 - 100,(2009).

[10] Hua,"Wiener and Schultz molecular topological indices of graphs with specified cut edges", MATCH Commune. Math. Compute. Chem.61 643- 651, (2009).

[11] H. Wang, "The external values of the Wiener index of a tree with given degree sequence", Discrete Applied Mathematics.156 2647-2654,(2009).

[12] H. Wiener, "Structural Determination of Paraffin Boiling Points", J. Amer. Chem Soc. , 69, 17-20,(1947).

[13] H.Y. Zhu, D. Klein, I. Lukovits," Extensions of the Wiener Number ",J. Chem. Inf. Compute. Sci. , 36, 420-428,(1996).

[14] J. Riordan and N. J. A. Sloane," The enumeration of rooted trees by total height", J. Austral. Math. Soc., 10:278-282,(1969).

[15] J. W. Moon," On the expected distance from the centroid of a tree", Ars Combin. 20(A):2637-276, 1985. Tenth British combinatorial conference Glasgow,(1985).

[16] Leon Ramzews and Benedikt Stuer,"Simply Generated Unrooted Plane Trees", Alea, Lat. Am. J. Probab. Math. Stat,16, 333-359,(2019).

[17] N. Sabine,"The Wiener index of a graph", thesis of Graz University of Technology ,(2010).
[18] R. C. Entringer, A. Meir, J. W. Moon, and L. A. Szekely," The Wiener index of trees from certain families", Australas. J. Combin., 10:211- 224,(1994).
[19] R. Shi,"The average distance of trees",Systems Sci. Math. Sci., 6:18- 24,(1993).
[20] R. Sridharamurthy, A. Kamakshidasan, and V. Natarajan,"Edit Dis- tances for Comparing Merge Trees", in Ieee SciVis Posters, (2017).
[21] S. C. Li, M. Zhang, G. H. Yu, L. H. Feng,"On The extremal Values of The eccentric distance sum of trees" J. Math. Anal. Appl. 390, 99-112,(2012).
[22] Stephan G. Wagner," On the average Wiener index of degree-restricted trees", This work was supported by Austrian Science Fund project no. S-8307-MAT.
[23] V. A. Graovac and T. Pisanski,"On the Wiener index of a graph", J. Math. Chem.8, 53-62,(1991).
[24] V. Narayanan, D. M. Thomas, and V. Natarajan,"Distance Between Extreme Graphs", in Paci_c Vis, ,pp, 263-270,(2015).
[25] X. Y. Geng, S. C. Li, M. Zhang,"Extremal Values on The eccentric Distance Sum of Trees" Discr. Appl. Math. 161 2427-2439,(2013).