Wiener Indices of Binary Trees

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Abstract

One of the most widely known topological index is the Wiener index. The Wiener Index Conjecture states that all positive integer numbers except a finite set are the Wiener indices of some trees. We explore the Wiener indices of the binary trees. We present efficient algorithms for generating the Wiener indices of the binary trees. Based on experiments we strengthen the conjecture for the class of the binary trees.

Key-Words: Molecular graphs, topological indices, Wiener index.

1 Introduction

Molecules and molecular compounds are often modeled by *molecular graphs*. Topological indices of molecular graphs are one of the oldest and most widely used descriptors in quantitative structure activity relationships: Quantitative structure activity relationships (QSAR) is a popular computational biology paradigm in modern drug design [3, 11]. One of the most widely known topological descriptor [6, 9] is the *Wiener index* named after chemist Harold Wiener [13] who devised it and studied it 57 years ago. The Wiener index of a graph $G(V, E)$ is defined as

$$W(G) = \sum_{u,v \in V} d(u, v), \tag{1}$$

where $d(u, v)$ is the distance between vertices u and v.

A majority of the chemical applications of the Wiener index deal with chemical compounds that have acyclic organic molecules (see [8, 12] for details). The molecular graphs of these compounds are trees [7], see an example of a chemical compound in Fig. 1. Therefore most of the prior work on the Wiener indices deals with trees, relating the structure of various trees to their Wiener indices (asymptotic bounds on the Wiener indices of certain families of trees, expected Wiener indices of random trees etc.). For these reasons, we concentrate on the Wiener indices of trees as well (see Dobrynin *et al.* [4] for a recent survey).

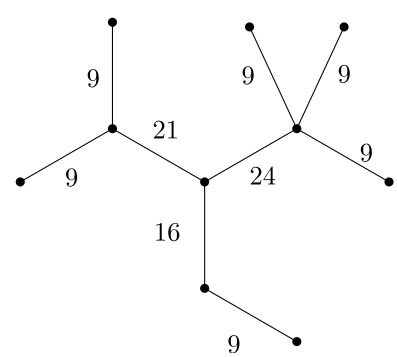

Figure 1: Carbon skeleton of 3-Ethyl-2,2,4-trimethylpentane. Its Wiener index 87, is the sum of the edge weights.

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Several papers address the question: What positive integer numbers can be Wiener indices of graphs of a certain type? The question is answered for general graphs and bipartite graphs [4]. The question is still open for trees.

Conjecture 1 [**Wiener Index Conjecture** [5, 10]] *Except for some finite set, every positive integer is the Wiener index of a tree.*

Lepović and Gutman [10] found the Wiener indices up to 1206 by enumerating all non-isomorphic trees of at most 20 vertices. They conjectured that 159 is the largest non-Wiener index of a tree. Goldman *et al.* [5] verified the conjecture for the Wiener indices up to 10^4. Recently Bespamyatnikh *et al.* [1] found a class of trees whose Wiener indices cover all numbers up to 10^8. Although their algorithm is very fast, the trees may have vertices of large degrees.

We define a *d-tree*, $d = 2, 3 \ldots$ as a rooted tree such that every node has degree at most d. Let $\mathcal{F}_d$ denote the family of all d-trees. $\mathcal{F}_d, d = 0, 1, 2 \ldots$ is a growing family of trees since

$$\mathcal{F}_0 \subset \mathcal{F}_1 \subset \mathcal{F}_2 \subset \ldots$$

Let $\mathcal{F}_d(n)$ denote the set of d-trees of size n. Let $W(\mathcal{F}_d)$ and $W(\mathcal{F}_d(n))$ denote the set of the Wiener indices of the trees in $\mathcal{F}_d$ and $\mathcal{F}_d(n)$, respectively. The family $\mathcal{F}_2$ contains trees that are paths. The Wiener index of a path with n vertices is $\binom{n+1}{3}$. Therefore the Wiener indices of trees of $\mathcal{F}_2$ cannot justify Conjecture 1. The question we address in this paper is the following. Is there an integer d such that the Wiener indices of trees of $\mathcal{F}_d$ can justify Conjecture 1? Our results suggest that such a number exists and, even more, that $d = 3$ is very likely to be the smallest degree of trees whose Wiener indices cover all sufficiently large integers.

We study the class of binary trees $\mathcal{F}_3$. There are only two non-isomorphic binary trees of size

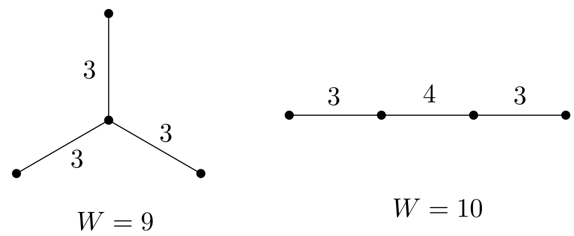

Figure 2: Two trees of $\mathcal{F}_3(4)$ and their Wiener indices.

4 depicted in Fig. 2. We present efficient algorithms for computing the Wiener indices of $\mathcal{F}_d(n)$. We implemented the algorithms and found all Wiener indices $W(\mathcal{F}_3)$ up to 150000. Our experiments allow us to suggest the following.

Conjecture 2 *Except for some finite set, every positive integer is the Wiener index of a binary tree.*

2 Preliminaries

Canfield *et al.* [2] applied a recursive approach for calculating the Wiener index of a tree. For a rooted tree T, we denoted by $l(T)$ the sum of the distances from the root v_{root} of T to all its vertices, $l(T) = \sum_{v \in T} d(v_{root}, v)$.

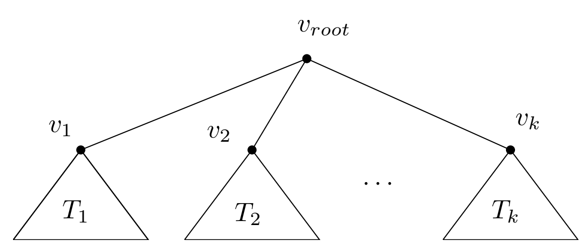

Figure 3: Recursive computation of the Wiener index.

Theorem 3 (Canfield *et al.* **[2])** *Let T be a tree of size n with the root v_{root} and let $v_i, 1 \leq i \leq k$ be the vertices adjacent to v_{root}. Let $T_i, 1 \leq i \leq k$ be the subtree of T rooted at v_i. Let n_i be the size of $T_i, 1 \leq i \leq k$, see Fig. 3.*

Then

$$W(T) = n(n-1) \tag{2}$$
$$+ \sum_{i=1}^{k} [W(T_i) + (n - n_i)l(T_i) - n_i^2]$$

$$l(T) = n - 1 + \sum_{i=1}^{k} l(T_i). \tag{3}$$

For an edge e of a tree T, let $w(e) = n_1(e)n_2(e)$ denote its *weight* where $n_1(e)$ and $n_2(e)$ are the sizes of two trees left after the removal of e, see Fig. 1 for example. The following formula was discovered by Wiener [13]

$$W(G) = \sum_{e \in T} n_1(e)n_2(e). \tag{4}$$

The formula for the Wiener index using edge weights is useful in practice when the Wiener index is calculated by hand. Figures 1 and 2 illustrate the edge weights in the graphs.

3 Algorithms and Experiments

Our algorithms for enumerating the Wiener indices are based on the algorithms by Goldman *et al.* [5] and Bespamyatnikh *et al.* [1]. These algorithms apply the dynamic programming technique.

Let T be a rooted binary tree. We encode it by the triple (n, l, w) where n is the size of T, l is $l(T)$ and $w = W(T)$. We compute lists $L(n), n = 1, 2, \ldots, N$ that store pairs (l, w) for all binary trees of size n. We store the pairs in $L(n)$ in the lexico-graphical order. This allows us to find a triple (n, l, w) in $O(\log M)$ time using the binary search where M is the total size of the lists $L(n)$.

The algorithm computes the list $L(n)$ as follows. For every pair n_1, n_2 such that $n_1 \leq n_2$ and $n_1 + n_2 = n - 1$, the algorithm checks every pair $(l_1, w_1) \in L(n_1)$ and every pair $(l_2, w_2) \in L(n_2)$. The resulting pair (l, w) can be found by Equation (2) and (3). The pseudo-code of the algorithm is shown in Appendix.

We implemented the above algorithm and run it for $n \leq 30$ only since the sizes of the lists $L(n)$ grow rapidly. Nevertheless, the largest non-Wiener index we found is 405. To conclude this we also compute the smallest Wiener index of the list $L(30)$ which is larger than 1000. The list of non-Wiener indices up to 405 is shown in Table 1.

This leads to the following conjecture.

Conjecture 4 *Except for 128 integer numbers shown in Table 1, every positive integer is the Wiener index of a binary tree.*

We modified the algorithm to be able to verify Conjecture 4 for large numbers. The idea is that we want to store not all pairs (l, w) in $L(n)$ so that the larger Wiener indices can be discovered. We developed several constraints that restrict the stored pairs (l, w). One of the constraints is the bound on the number of pairs (l, w) for the same value w. The constraints allow us to explore larger numbers. The best bound we found is 150000. In other words every number between 406 and 150000 is the Wiener index of a binary tree. This large interval supports Conjecture 4.

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Table 1: Table presenting a set of 128 integers that are not represented a Wiener index of a binary tree.

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A Appendix: The algorithm

Algorithm 1 WienerIndicesOfBinaryTrees

Require: An integer N, the maximum value of n.

Ensure: The lists $L(n)$ where $1 \leq n \leq N$.

An integer M, the maximum value of $\mathcal{W}(\mathcal{F}_d(n))$ over all $1 \leq n \leq N$.

The boolean list $W[0...M]$ whose i-th value is 1 if i is in the lists $L(n) 1 \leq n \leq N$; 0 otherwise.

```
L(0) = {0,0} and L(1) = {0,0} {Initialization}
for i = 1 to sizeofW[] do
  W[i] = 0
end for
for n = 2 to N do
  L(n) = ∅
  for n_1 = 0 to ⌊(n − 1)/2⌋ do
    n_2 = n − n_1 − 1
    for each (l_1, w_1) ∈ L(n_1) and each (l_2, w_2) ∈ L(n_2) do
      l = l_1 + l_2 + n − 1
      w = w_1 + l_1 + n_1 + w_2 + l_2 + n_2 + l_1 n_2 + l_2 n_1 + 2 n_1 n_2
      if (l, w) ∉ L(n) then
        insert (l, w) in L(n)
        W[w] = 1
        M = M + 1
      end if
    end for
  end for
end for
```