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Equiseparability on terminal Wiener index

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ABSTRACT

The aim of this work is to explore the properties of the terminal Wiener index, which was recently proposed by Gutman et al. (2004) [3], and to show the fact that there exist pairs of trees and chemical trees which cannot be distinguished by using it. We give some general methods for constructing equiseparable pairs and compare the methods with the case for the Wiener index. More specifically, we show that the terminal Wiener index is degenerate to some extent.

1. Introduction

There are many chemical indices that have been proposed as molecular structure descriptors so far; one of the oldest and most well studied chemical indexes is the *Wiener index* which was given by Wiener [1] in 1947. It can be expressed as

$$W(G) = \sum_{1\le i<j\le n} d(v_i, v_j) \tag{1}$$

where $d(v_i, v_j)$ is the distance between vertices v_i and v_j in a graph G, and the summation goes over all pairs of vertices of the given graph. For trees, Wiener obtained a very useful formula for calculating the Wiener index:

$$W(T) = \sum_{e\in T} n_1(e|T)\cdot n_2(e|T) \tag{2}$$

where $n_1(e|T)$ and $n_2(e|T)$ are the numbers of vertices of T lying on either side of e. The summation on the right-hand side of the equation goes over all edges of the tree T. Obviously, if the tree T has n vertices, then for all of its edges,

$$n_1(e|T) + n_2(e|T) = n.$$

On the basis of Wiener index, a general index called the *variable Wiener index* has been proposed [2,3]:

$$W_\lambda(T) = \sum_{e\in T} [n_1(e|T)\cdot n_2(e|T)]^\lambda \tag{3}$$

where λ is an adjustable parameter.

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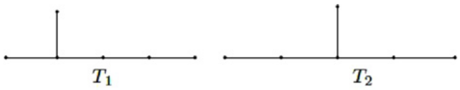

Fig. 1. *Two trees* with the same variable terminal Wiener index.

Definition 1 ([4]). Assuming that $n_1(e|T) \leq n_2(e|T)$, two trees T' and T'' of order n are said to be *equiseparable* if their edges $e'_1, e'_2, \dots, e'_{n-1}$ and $e''_1, e''_2, \dots, e''_{n-1}$ can be labeled such that the equality $n_1(e'_i|T') = n_1(e''_i|T'')$ holds for all $i = 1, 2, \dots, n-1$.

The Wiener index has been extensively used in computational biology, preliminary screening of drugs and complex networks. For example, it is a measurement of the average distance in network [5,6]. In the design of economical networks, spanning trees of connected graphs with the smallest Wiener index are very important in practice [7]. In chemistry, the Wiener index measures the van der Waals surface area of an alkane molecule, which explains the correlations found between W and a great variety of physico-chemical properties of alkanes [8]. But if two or more chemical trees are equiseparable, then those compounds will have similar physico-chemical properties which cannot be distinguished by means of the Wiener index. This is a main drawback of many chemical index structure descriptors.

Gutman et al. [4] pointed out that there exist pairs of isomeric alkanes whose variable Wiener indexes coincide for all values of the parameter λ. Some former studies [4,9] showed how to construct such equiseparable chemical trees. From another point of view, Vukičević and Gutman [10] gave a proof that almost all trees and chemical trees[2] have equiseparable mates.

In [11], Smolenskii et al. made use of terminal distance matrices to encode molecular structures. The proposed reduced vector is less degenerate than for some other molecular codes. On the basis of those applications, Gutman et al. [12] proposed the concept of the *terminal Wiener index*, which is equal to the summation of the distances between all pairs of pendent vertices[3] of trees, i.e.

$$TW(T) = \sum_{1 \leq i < j \leq k} d(v_i, v_j) \tag{4}$$

where v_i and v_j are pendent vertices of tree T, $d(v_i, v_j)$ is the distance between them, and the sum goes over all pairs of such pendent vertices.

Using a proof similar to that of (2), Gutman found another way to calculate the terminal Wiener index:

$$TW(T) = \sum_{e \in T} p_1(e|T) \cdot p_2(e|T) \tag{5}$$

where $p_1(e|T)$ and $p_2(e|T)$ are the numbers of pendent vertices of T lying on either side of e, and the summation embraces all the $n-1$ edges of T. We will use $p_1(e), p_2(e)$ instead of $p_1(e|T), p_2(e|T)$ when there is no confusion.

We define the variable terminal Wiener index, similarly to the Wiener index, in order to achieve more molecular structure descriptive power.

Definition 2. The variable terminal Wiener index is defined as follows:

$$TW_\lambda(T) = \sum_{e \in T} [p_1(e) \cdot p_2(e)]^\lambda \tag{6}$$

where λ is an adjustable parameter.

Unfortunately, with this more powerful index, there still exist pairs of trees and chemical trees whose variable terminal Wiener indexes coincide for all values of the parameter λ. We can see this from the example in Fig. 1, where T_1 and T_2 have the same variable terminal Wiener index, $5 \cdot 2^\lambda$.

On the basis of this fact, we define equiseparability w.r.t. the terminal Wiener index.

Definition 3. Assuming that $p_1(e) \leq p_2(e)$, two trees T' and T'' of order n with the same number of pendent vertices are said to be *equiseparable* w.r.t. the terminal Wiener index if their edges $e'_1, e'_2, \dots, e'_{n-1}$ and $e''_1, e''_2, \dots, e''_{n-1}$ can be labeled such that the equality $p_1(e'_i|T') = p_1(e''_i|T'')$ holds for all $i = 1, 2, \dots, n-1$.

We see that trees equiseparable w.r.t. the terminal Wiener index have equal Wiener indices and variable terminal Wiener indices (for all λ).

In Section 2, we explore different rules for constructing equiseparable trees w.r.t. the Wiener index and terminal Wiener index. In Section 3, we give a formal proof of the fact that the terminal Wiener index is degenerate like the Wiener index.

[2] A tree is a chemical tree if its maximum degree is at most 4.

[3] In this work, pendent vertices indicate leaves of the tree.

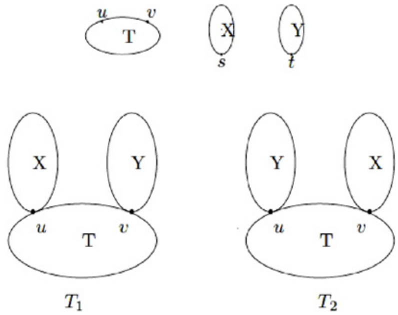

Fig. 2. Equiseparable chemical trees w.r.t. Wiener index constructed by the method in Theorem 1.

2. Rules for constructing equiseparable trees with respect to the terminal Wiener index

First, we show that the methods for constructing equiseparable trees w.r.t. the Wiener index in [4,9] can be extended to construct equiseparable trees w.r.t. the terminal Wiener index.

In [4], Gutman obtained some rules for constructing equiseparable chemical trees w.r.t. the Wiener index. But they are in fact special cases of the method obtained in [9], which can be stated as:

Theorem 1 (*[9]*)**.** *Let T, X and Y be arbitrary trees, each with more than two vertices. Let the tree T_1 be obtained from T by identifying the vertices u and s, and by identifying the vertices v and t. Let T_2 be obtained from T by identifying the vertices u and t, and by identifying the vertices v and s. Then if X and Y have equal numbers of vertices, the trees T_1 and T_2 are equiseparable. See Fig. 2.*

If we revise the condition felicitously, then Theorem 1 can be extended to constructing equiseparable trees w.r.t. the terminal Wiener index.

Theorem 2. *Let trees T_1 and T_2 be constructed in the same way as they are in Fig. 2. If $p_x - p_s = p_y - p_t$, then the trees T_1 and T_2 are equiseparable w.r.t. the terminal Wiener index. p_x and p_y denote the number of pendent vertices of fragments X and Y, respectively. p_s is equal to 1 if s is a pendent vertex of X; otherwise it is equal to 0. p_t is defined similarly to p_s.*

Proof. We prove this by classifying the edges of T_1 and T_2 into four types with each type of edge satisfying Definition 3.

(1) For edges belonging to T, lying on the same side of u and v, for example, edge e' of T_1 and e'' of T_2, both lying on the left of u: We have $p_1(e'|T_1) = p_1(e''|T_2) = p_1(e|T)$, $p_2(e'|T_1) = p_2(e''|T_2) = p_2(e|T) + p_x + p_y - k$, where k is a constant which equals the number of pendent vertices among $\{u, v, s, t\}$. So such edges can be labeled such that $p_1(e'|T_1) = p_1(e''|T_2)$ always holds. The same applies to edges lying on the right of v.
(2) For edges belonging to X: Obviously there is a bijection between the edges of fragment X of T_1 and the edges of fragment X of T_2, so such edges can also be labeled such that $p_1(e'|T_1) = p_1(e''|T_2)$ always holds.
(3) For edges belonging to Y: This is the same as case (2).
(4) For edges belonging to T, lying between the vertices u and v: According to whether vertices u, v, s, t are pendent vertices of their corresponding fragments, this case can be divided into $2^4 = 16$ subcases. We only check three typical subcases here; the others can be proved similarly.
   (4.1) None of them is a pendent vertex.
   Then we have $p_1(e'|T_1) = p_1(e|T) + p_x$, $p_2(e'|T_1) = p_2(e|T) + p_y$ and $p_1(e''|T_2) = p_1(e|T) + p_y$, $p_2(e''|T_2) = p_2(e|T) + p_x$. Combining with $p_s = 0$ and $p_t = 0$, we get that the equality $p_x - p_s = p_y - p_t$ implies that the edges lying between u and v satisfy Definition 3.
   (4.2) One of them is a pendent vertex; for example, s is a pendent vertex of X.
   Then we have $p_1(e'|T_1) = p_1(e|T) + p_x - 1$, $p_2(e'|T_1) = p_2(e|T) + p_y$ and $p_1(e''|T_2) = p_1(e|T) + p_y$, $p_2(e''|T_2) = p_2(e|T) + p_x - 1$. Combining with $p_s = 1$ and $p_t = 0$, we get that the equality $p_x - p_s = p_y - p_t$ implies that the edges lying between u and v satisfy Definition 3.
   (4.3) Two of them are pendent vertices; for example, s is a pendent vertex of X while v is a pendent vertex of T.
   Then we have $p_1(e'|T_1) = p_1(e|T) + p_x - 1$, $p_2(e'|T_1) = p_2(e|T) + p_y - 1$ and $p_1(e''|T_2) = p_1(e|T) + p_y$, $p_2(e''|T_2) = p_2(e|T) + p_x - 2$. Combining with $p_s = 1$ and $p_t = 0$, we get that the equality $p_x - p_s = p_y - p_t$ implies that the edges lying between u and v satisfy Definition 3.

After checking all 16 subcases we get that edges lying between u and v can be labeled such that $p_1(e'|T_1) = p_1(e''|T_2)$ always holds.

Aggregating these four cases, we can see that if $p_x - p_s = p_y - p_t$, then $p_1(e'_i|T') = p_1(e''_i|T'')$ holds for all $i = 1, 2, \ldots, n-1$, which implies that trees T_1 and T_2 are equiseparable.

On the other hand, trees being equiseparable w.r.t. the Wiener index does not imply that they are equiseparable w.r.t. the terminal Wiener index, since the terminal Wiener index is the sum of the distances between all pairs of pendent vertices but

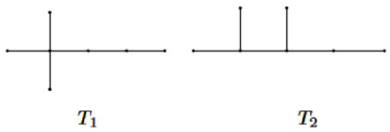

Fig. 3. Example of trees equiseparable w.r.t. Wiener index but not equiseparable w.r.t terminal Wiener index.

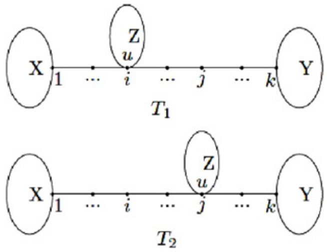

Fig. 4. Equiseparable trees w.r.t. terminal Wiener index constructed by the method in Theorem 3.

not pairs of vertices. For example, the trees T_1 and T_2 in Fig. 3 are equiseparable w.r.t. the Wiener index but not equiseparable w.r.t. the terminal Wiener index. So, it is worth finding some general rules for constructing equiseparable trees w.r.t the terminal Wiener index only.

The following theorem and corollary provide rules for constructing equiseparable trees w.r.t. the terminal Wiener index but not the Wiener index. □

Theorem 3. *Let Z be an arbitrary tree; u is a vertex of Z, tree T_1 is obtained by identifying the vertices u and i, and T_2 is obtained by identifying the vertices u and j. If X and Y have equal numbers of pendent vertices, then the trees T_1 and T_2 are equiseparable. See Fig. 4.*

Proof. Suppose the numbers of pendent vertices of fragments X, Y and Z are p_x, p_y and p_z, respectively. If u is a pendent vertex of Z then k is equal to 1; otherwise k is equal to 0.

For each pair of edges e' of T_1 and e'' of T_2 which are lying on the left of vertex i, the numbers of pendent vertices sited on the two sides of these edges are p_x and $p_y + p_z - k$, respectively. So the edges lying on the left of vertex i can be labeled such that $p_1(e'_i|T_1) = p_1(e''_i|T_2)$ always holds.

The same applies to the edges which are lying on the right of vertex j and belong to fragment Z, so we only need to consider the edges lying between vertices i and j.

For the edge e' of T_1 which is lying between i and j, the numbers of pendent vertices sited on the two sides of e' are $p_x + p_z - k$ and p_y; for the edge e'' of T_2 which is lying between i and j, the numbers of pendent vertices sited on the two sides of e'' are p_x and $p_y + p_z - k$.

Since $p_x = p_y$, we can label the edges $e'_1, e'_2, \ldots, e'_{n-1}$ of T_1 and $e''_1, e''_2, \ldots, e''_{n-1}$ of T_2 such that the equality $p_1(e'_i|T_1) = p_1(e''_i|T_2)$ holds for all $i = 1, 2, \ldots, n-1$. Therefore T_1 and T_2 are equiseparable w.r.t. the terminal Wiener index.

Note that since $TW(T)$ only depends on the distance between pairs of pendent vertices, the position of fragment Z can be arbitrary, lying on the path from 1 to k. But for the Wiener index, things are different. Fragments X and Y having equal numbers of vertices is not sufficient for equiseparability when fragment Z is moving arbitrarily between vertex i and j; we can see this from the two trees in Fig. 1.

Theorem 3 can be extended to the circumstances where there is more than one fragment on the path from 1 to k. □

Corollary 1. *If the fragments X and Y have equal numbers of pendent vertices, with the fragments $Z_1, Z_2, \ldots, Z_t$ moving without changing the distance between them, then the resulting two (chemical) trees are equiseparable w.r.t. the terminal Wiener index. See Fig. 5 for an illustration.*

The proof of Corollary 1 is omitted here.

3. Degeneracy of terminal Wiener indexes

Vukičević and Gutman [10] developed a powerful technique in order to prove that almost all trees and chemical trees have equiseparable mates w.r.t. the Wiener index; the proof of the chemical tree case is omitted since it is more complicated than the case of trees. In this section, we show that the terminal Wiener index is degenerate by proving that almost all chemical trees have equiseparable mates.

Let T be an n-vertex tree with k $(2 \leq k \leq n-1)$ pendent vertices; $e_1, e_2, \ldots, e_{n-1}$ are its edges. We can relate T to a sequence $\varphi(T)$ as follows. Assume that for each edge e_i of the tree T, $p_1(e_i|T) \leq p_2(e_i|T)$. Let $t_j(T)$, among the numbers $p_1(e_i|T)$, $i = 1, 2, \ldots, n-1$, be equal to j, $j = 1, \ldots, \lfloor k/2 \rfloor$. In other words, $t_j(T)$ is the number of edges such that the

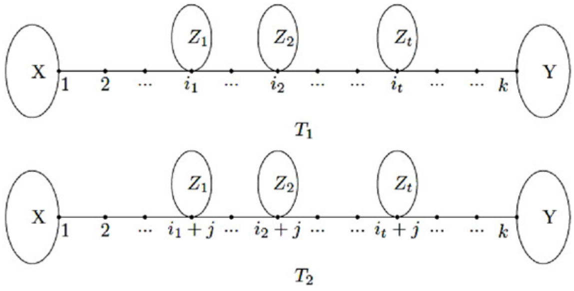

Fig. 5. Equiseparable trees w.r.t. terminal Wiener index constructed by the method in Corollary 1.

number of pendent vertices lying on one side of e_i, where this is less than the number lying on the other side, is equal to j. Then the ordered $\lfloor k/2 \rfloor$-tuple of integers (either positive or zero)

$$\varphi(T) = (t_1(T), t_2(T), \ldots, t_{\lfloor k/2 \rfloor}(T))$$

is called the *separation sequence* of T.

Remark. (i) The separation sequence $\varphi(T) = (t_1(T), t_2(T), \ldots, t_{\lfloor k/2 \rfloor}(T))$ does not depend on the labeling of the edges of T.

(ii) Since an n-vertex tree T with k pendent vertices has $n-1$ edges, $\sum_{j=1}^{\lfloor k/2 \rfloor} t_j(T) = n-1$.

(iii) Let T_1 and T_2 be two n-vertex trees with k pendent vertices. By Definition 3, T_1 and T_2 are equiseparable if and only if $\varphi(T_1) = \varphi(T_2)$, i.e., two n-trees with the same number of pendent vertices are equiseparable if and only if their separation sequences coincide.

Theorem 4. *The terminal Wiener index is degenerate in the sense that almost all chemical trees have equiseparable mates.*

Proof. Let CT_n be the set of chemical trees of order n, and U_n and CU_n the sets of trees and chemical trees of order n having no equiseparable mates, respectively. Let $|S|$ denote the number of elements in set S. Then what we need to prove is

$$\lim_{n\to\infty} \frac{|CU_n|}{|CT_n|} = 0.$$

We first give an upper bound of $|CU_n|$. It is obvious that $|CU_n| \leq |U_n|$.

Let $U_{n,k}$ be the set of trees with n vertices and k pendent vertices having no equiseparable mates. Then $U_n = U_{n,2} \cup U_{n,3} \cup \cdots \cup U_{n,\lfloor k/2 \rfloor}$, and $|U_n| \leq \sum_{k=2}^{n-1} |U_{n,k}|$.

Let A be the set of ordered $\lfloor k/2 \rfloor$-tuples of nonnegative integers whose sum is equal to $n-1$. Then $|A| = \binom{\lfloor k/2 \rfloor + n - 2}{\lfloor k/2 \rfloor - 1}$ according to a standard result of combinatorics.

Now, let $\varphi : U_{n,k} \to A$ and $\varphi(T)$ be the separation sequence of T for any $T \in U_{n,k}$. By Remark (iii), φ is injective, and we have $|U_{n,k}| \leq |A| = \binom{\lfloor k/2 \rfloor + n - 2}{\lfloor k/2 \rfloor - 1}$.

So, we have an upper bound on $|U_n|$:

$$|U_n| \leq \sum_{k=2}^{n-1} |U_{n,k}| \leq \sum_{k=2}^{n-1} \binom{\lfloor k/2 \rfloor + n - 2}{\lfloor k/2 \rfloor - 1}$$
$$= \begin{cases} 2\displaystyle\sum_{k=1}^{(n-3)/2} \binom{k+n-2}{k-1} + \binom{\frac{n-1}{2} + n - 2}{\frac{n-1}{2} - 1} & \text{for } n \text{ is odd;} \\ 2\displaystyle\sum_{k=1}^{\frac{n}{2}-1} \binom{k+n-2}{k-1} & \text{for } n \text{ is even} \end{cases}$$

and by employing a combinatorial recursive formula, we get

$$|CU_n| \leq |U_n| \leq \begin{cases} 2\displaystyle\sum_{k=1}^{(n-1)/2} \binom{k+n-2}{k-1} \\ 2\displaystyle\sum_{k=1}^{\frac{n}{2}-1} \binom{k+n-2}{k-1} \end{cases} \leq \begin{cases} 2\dbinom{\frac{3n-3}{2}}{\frac{n-3}{2}} & \text{for } n \text{ is odd;} \\ 2\dbinom{\frac{3n-4}{2}}{\frac{n-4}{2}} & \text{for } n \text{ is even} \end{cases}$$

For $|CT_n|$, Otter [13] obtained an asymptotic value for the number of trees $T_{n,m}$ of order n and maximum degree m, i.e., for $3 \le m < \infty$,

$$|T_{n,m}| \sim \frac{\beta^3 \cdot a_{m-3}}{4\sqrt{\pi} \cdot \alpha^{-2.5}} \frac{\alpha^n}{n^{2.5}}$$

where α, β and a_{m-3} are constant for any fixed m. Specifically, for $m = 4$, i.e., for chemical trees, $\alpha = 2.81546$, $\beta = 3.08039$, $a_1 = 2.11742$. Hence we get

$$|CT_n| \sim k \cdot \frac{\alpha^n}{n^{2.5}}, \quad k = 0.65632, \ \alpha = 2.81546$$

Obviously, $|CT_n|$ is exponential on n. Then we have

$$\lim_{n\to\infty} \frac{|CU_n|}{|CT_n|} = 0. \quad \square$$

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