Terminal Wiener Index of
Star-Tree and Path-Tree

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Abstract

Quantitative Structure Activity (resp. property) Relationships (QSAR/QSPR), are two studies based on the Modeling Methods, which starts with the representation of the input data by using of molecular descriptors, so called the topological indices. A topological index is the graph invariant number calculated from a graph representing a molecule, offering an effective way to measure molecular branching, and molecular similarity. The Terminal Wiener index $TW(T)$ of a tree $T$, is one of the recent topological indices, that has been put forward and investigated in several published articles. In this paper, we give theoretical results for calculating the Terminal Wiener index for some composed trees, and some examples of its results.

Mathematics Subject Classification: 05C10, 05C12
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I Introduction

The study of Quantitative Structure-Activity Relationships (QSAR) and Quantitative Structure-Property Relationships (QSPR) are mathematical models, based on research of the relationship between structure and activity (property) of a compound or molecule, in other words, in a QSAR/QSPR study an attempt is made to relate the structure of a molecule to a biological activity or a property by means of statistical tools.

Developing a QSAR/QSPR models, starts with the collection of reliable data. Following that, development a set of molecular descriptors that characterize the structures of the collected molecules, the molecular descriptors describes the important information of the molecules, and are partitioned into classes: 1D-descriptors, 2D-descriptors, and 3D-descriptors. Tools of data analysis are then used to select of the most informative descriptors. Subsequently, for tuning and validation of the QSAR/QSPR models, the full data set is divided into a training set and a testing set. During the training step, various modeling methods like Multiple Linear Regression, Logistic Regression, and Neural Networks, are used to build models that describe the relation between structure and activity (property). The resulting model is then validated by a testing set to ensure that the model is appropriate and useful.

In this paper we are limited to the classe of 2D-descriptors, Known as topological indices, which turned out to be powerful for modeling and predicting the properties for various molecular structures, and consider the structure of the compound as a graph, they can be easily calculated from the molecular graph.

II Preliminary Notes

A graph $G = (V, E)$, is a pair of two sets, $V = V(G)$ is the set of vertices of $G$, and $E = E(G)$ the set of edges of $G$. The degree $\deg(v)$ of a vertex $v$ is equal to the number of edges incident on $v$. We say a vertex is pendent if its degree is unity. The distance $d(u,v)$ between two vertices $u$ and $v$ denote the length of the shortest path connecting these two vertices. If $G$ is a molecular graph then $V(G)$ represents the set of atoms in $G$, and $E(G)$ represents the connection between pairs of atoms.

The Wiener index is one of the most popular and well studied topological index, it was introduced by H. Wiener [11] in 1947. Wiener index $W(G)$ of
a graph $G$, is the sum of the distances between all pairs of vertices in $V(G)$:
$$W(G) = \sum_{\{u,v\} \subseteq V(G)} d(u, v),$$
and the Wiener index of a vertex $v$ in $G$ is defined as:
$$w(v, G) = \sum_{u \subseteq V(G)} d(v, u).$$

In the last years a numerous modification and extensions of the Wiener index was proposed and studied by mathematical chemists, these include the Terminal Wiener index $\mathcal{TW}(T)$, proposed by the authors of [6,7]. The Terminal Wiener index $\mathcal{TW}(T)$ of a tree $T$, equal to the sum of the distances between all pairs of pendent vertices $V_p(T) \subseteq V(T)$ of the tree $T$:
$$\mathcal{TW}(T) = \sum_{\{u,v\} \subseteq V_p(T)} d(u, v),$$
and the distance between a vertex $S$ and pendent vertices of $T$ is defined as: $tw(S, T) = \sum_{u \subseteq V_p(T)} d(S, u)$. For more details on Terminal Wiener index of trees, see [3,4,5].

The authors of [6], have been proposed a formula to calculate efficiently the Terminal Wiener index:
$$\mathcal{TW}(T) = \sum_e p_1(e/T)p_2(e/T)$$
$p_1(e/T)$ and $p_2(e/T)$ are the number of pendent vertices of $T$, lying on the two sides of the edge $e$, with the summation includes all the $n - 1$ edges of $T$. In should be noted that, if $p$ is the number of pendent vertices of the tree $T$, then for any edge $e$ we have: $p_1(e/T) + p_2(e/T) = p$.

III Main Results

In the preceding paper [12] we presented formula for the Wiener and Terminal Wiener indices of some rooted trees, and according to the results presented in the article [1], We are going to show in this section the theoretical results for calculating the Terminal Wiener index for some composed trees.

Composed tree $\mathcal{T}_N$, is a tree composed of $N$ trees $T_{n_i}$ of order $n_i$, connected to each others by a vertex $S$ (i.e: the Star-Tree), or those $T_{n_i}$ are connected by a set of vertices $S_i$ for $i = \{1, 2, ..., N - 1\}$ (i.e: the Path-Tree).

III.1 Star-Tree

A Star-Tree $\mathcal{T}_N$ is a tree composed of $N$ trees $T_{n_i}$, each of them is of order $n_i$, and have $p_i$ pendent vertices, for $i = \{1, 2, ..., N\}$. the trees $T_{n_i}$ are connected by a common vertex $S$. (see Figure 1).

We interested in the case where $S$ is a pendent vertex of all the trees $T_{n_i}$ before the connection.

Theorem 1. Let $\mathcal{T}_2$ a Star-Tree composed of two trees $T_{n_1}$ and $T_{n_2}$ of order $n_1$ and $n_2$, and have $p_1$ and $p_2$ pendent vertices respectively. The two trees are
Figure 1: Star-Trees $T_2 : T_{n_1}.T_{n_2}$ and $T_N : T_{n_1}.T_{n_2}$. . . . $T_{n_N}$.

connected by a common pendent vertex $S$, (see Figure 1).
The Terminal Wiener index of the Tree $T_2$ is computed as:

$$TW(T_2) = TW(T_{n_1}) + TW(T_{n_2}) + (p_2 - 2)tw(S, T_{n_1}) + (p_1 - 2)tw(S, T_{n_2}) \quad (1)$$

Proof. By applying the definition of the Terminal Wiener we have:

$$TW(T_2) = \sum_{(u, v) \subseteq V_p(T_2)} d(u, v)$$

$$= \sum_{(u, v) \subseteq V_p(T_{n_1})} d(u, v) + \sum_{(u, v) \subseteq V_p(T_{n_2})} d(u, v) + \sum_{u \subseteq V_p(T_{n_1})} \sum_{v \subseteq V_p(T_{n_2})} d(u, v)$$

or:

$$\sum_{u \subseteq V_p(T_{n_1})} \sum_{v \subseteq V_p(T_{n_2})} d(u, v) = \sum_{u \subseteq V_p(T_{n_1})} \sum_{v \subseteq V_p(T_{n_2})} \left[ d(u, S) + d(S, v) \right]$$

then:

$$TW(T_2) = TW(T_{n_1}) - \sum_{u \subseteq V_p(T_{n_1})} d(u, S) + TW(T_{n_2}) - \sum_{v \subseteq V_p(T_{n_2})} d(S, v) +$$

$$+ \sum_{u \subseteq V_p(T_{n_1})} \sum_{v \subseteq V_p(T_{n_2})} d(u, S) + \sum_{u \subseteq V_p(T_{n_1})} \sum_{v \subseteq V_p(T_{n_2})} d(S, v)$$

$$= TW(T_{n_1}) + TW(T_{n_2}) + (p_2 - 2) \sum_{u \subseteq V_p(T_{n_1})} d(u, S) +$$

$$(p_1 - 2) \sum_{v \subseteq V_p(T_{n_2})} d(S, v)$$

which then explicitly yields Equation (1).

**Theorem 2.** Let $T_N$ a Star-Tree composed of $N$ trees $T_{n_i}$ of order $n_i$, and have $p_i$ pendent vertices, for $i = \{1, 2, ..., N\}$. The trees $T_{n_i}$ are connected by
a common pendent vertex $S$.

The Terminal Wiener index of the tree $T_N$ is computed as:

$$\mathcal{TW}(T_N) = \sum_{i=1}^{N} \mathcal{TW}(T_{n_i}) + \sum_{i=1}^{N-1} \sum_{j=i+1}^{N} [p_i \, tw(S, T_{n_j}) + p_j \, tw(S, T_{n_i})] - 
\sum_{i=1}^{N} tw(S, T_{n_i}) \tag{2}$$

Proof. By applying the definition of the Terminal Wiener we have:

$$\mathcal{TW}(T_N) = \sum_{\{u,v\} \subseteq V_p(T_N)} d(u, v)$$

$$= \sum_{\{u,v\} \subseteq V_p(T_{n_1})} d(u, v) + \sum_{\{u,v\} \subseteq V_p(T_{n_N})} d(u, v) + \sum_{u \subseteq V_p(T_{n_1}) \cap v \subseteq V_p(T_{n_2})} d(u, v) + \sum_{u \subseteq V_p(T_{n_1}) \cap v \subseteq V_p(T_{n_N})} d(u, v) + \sum_{u \subseteq V_p(T_{n_2}) \cap v \subseteq V_p(T_{n_3})} d(u, v) + \sum_{u \subseteq V_p(T_{n_2}) \cap v \subseteq V_p(T_{n_N})} d(u, v) + \cdots$$

$$= \sum_{i=1}^{N} \mathcal{TW}(T_{n_i}) + \sum_{i=1}^{N-1} \sum_{j=i+1}^{N} \left( \sum_{u \subseteq V_p(T_{n_i}) \cap v \subseteq V_p(T_{n_j})} d(u, v) \right) - \sum_{i=1}^{N} \sum_{u \subseteq V_p(T_{n_i})} d(u, S)$$

We have:

$$\sum_{u \subseteq V_p(T_{n_i}) \cap v \subseteq V_p(T_{n_j})} d(u, v) = (p_j - 1) \sum_{u \subseteq V_p(T_{n_j})} d(u, S) + (p_i - 1) \sum_{v \subseteq V_p(T_{n_i})} d(S, v)$$

Which yield the Equation (2). \qed

Corollary 1. Let $T_N$ a Star-Tree composed of the same $N$ trees $T_n$ of order $n$, and have $p$ pendent vertices. The trees $T_n$ are connected by a common pendent vertex $S$. The Terminal Wiener index of the Tree $T_N$ is computed as:

$$\mathcal{TW}(T_N) = N \, \mathcal{TW}(T_n) + N[(N - 1)p - N] \, tw(S, T_n) \tag{3}$$
Proof. The trees $T_n$ have the same number of vertices $n$, and pendent vertices $p$, then we have:

\[
T_{n_i} = T_{n_j} = T_n \\
p_i = p_j = p \\
tw(S, T_{n_i}) = tw(S, T_{n_j}) = tw(S, T_n)
\]

We apply (4) in the formula (2), then we get the result presented in Equation (3).

### III.2 Path-Tree

A Path-Tree $\mathcal{T}_N$ is a tree composed of $N$ trees $T_{n_i}$, each of them is of order $n_i$, and have $p_i$ pendent vertices, for $i = \{1, 2, ..., N\}$. The trees $T_{n_i}$ are connected by a set of vertices $S_i$ for $i = \{1, 2, ..., N - 1\}$, or a set of edges $\{S_i, S_{i+1}\}$ for $i = \{1, 2, ..., N\}$.

We are interested to the theoretical treatment of the Path-Tree, composed of $N$ trees $T_{n_i}$ connected to each others by introducing a set of edges $\{S_i, S_{i+1}\}$. (see Figure 2).

![Figure 2: Path-Tree $\mathcal{T}_N : T_{n_1} - T_{n_2} - ... - T_{n_N}$.](image)

**Lemma 1.** Let $\mathcal{T}_2$ a Path-tree composed of two trees $T_{n_1}$ and $T_{n_2}$ of order $n_1$ and $n_2$, and have $p_1$ and $p_2$ pendent vertices respectively. The two trees are connected by introducing an edge $\{S_1, S_2\}$.

- In the case of $S_1 \in V(T_{n_1})$ and $S_2 \in V(T_{n_2})$, the Terminal Wiener index of the Tree $\mathcal{T}_2$ is:

\[
\mathcal{TW}(\mathcal{T}_2) = \mathcal{TW}(T_{n_1}) + \mathcal{TW}(T_{n_2}) + p_2 tw(S_1, T_{n_1}) + p_1 tw(S_2, T_{n_2}) + p_1 p_2
\]

- If $S_1 \in V_p(T_{n_1})$ and $S_2 \in V_p(T_{n_2})$, then the Terminal Wiener index of the Tree $\mathcal{T}_2$ is computed as:

\[
\mathcal{TW}(\mathcal{T}_2) = \mathcal{TW}(T_{n_1}) + \mathcal{TW}(T_{n_2}) + (p_2 - 2)tw(S_1, T_{n_1}) + (p_1 - 2)tw(S_2, T_{n_2}) + (p_1 - 1)(p_2 - 1)
\]
Proof. The same manner applied in the proof of Theorem 1.

Theorem 3. Let \( T_N \) a Path-tree composed of \( N \) trees \( T_{n_i} \) of order \( n_i \), and have \( p_i \) pendent vertices, for \( i = \{1, 2, ..., N\} \). The trees are connected by introducing a set of edges \( \{S_i, S_{i+1}\} \), for \( i = \{1, 2, ..., N\} \).

- If \( S_i \in V(T_{n_i}) \), the Terminal Wiener index of the tree \( T_N \) is:

\[
TW(T_N) = \sum_{i=1}^{N} TW(T_{n_i}) + \sum_{i=1}^{N-1} \left[ p_i tw(S_{i+1}, T_{n_{i+1}}) + p_{i+1} tw(S_i, T_{n_i}) + p_i p_{i+1} \right] + \\
\sum_{i=1}^{N-2} \sum_{j=i+2}^{N} \left[ p_j tw(S_i, T_{n_i}) + p_i tw(S_j, T_{n_j}) + (j-i)p_i p_j \right]
\]

(7)

- If \( S_i \in V_p(T_{n_i}) \), the Terminal Wiener index of the tree \( T_N \) is:

\[
TW(T_N) = \sum_{i=1}^{N} TW(T_{n_i}) + \sum_{i=1}^{N-1} \left[ (p_i - 1) tw(S_{i+1}, T_{n_{i+1}}) + (p_{i+1} - 1) tw(S_i, T_{n_i}) \right] + \\
\sum_{i=1}^{N-2} \sum_{j=i+2}^{N} \left[ (p_j - 1) tw(S_i, T_{n_i}) + (j-i)(p_i - 1)(p_j - 1) \right] - \sum_{i=1}^{N} tw(S_i, T_{n_i})
\]

(8)

Proof. Following the way of proof applied in Theorem 2.

Corollary 2. Let \( T_N \) a Path-Tree composed of the same \( N \) trees \( T_n \) of order \( n \), and have \( p \) pendent vertices. The trees \( T_n \) are connected by a set of edges \( \{S_i, S_{i+1}\} \).

- If \( S_i \in V(T_n) \), the Terminal Wiener index of the tree \( T_N \) is:

\[
TW(T_N) = N \ TW(T_n) + pN(N-1) tw(S_1, T_n) + \frac{N(N^2 - 1) - p^2}{6}
\]

(9)

- If \( S_i \in V_p(T_n) \), then:

\[
TW(T_N) = N \ TW(T_n) + [N(N-1)(p-1)-N] tw(S_1, T_n) + \frac{N(N^2 - 1)(p-1)^2}{6}
\]

(10)
Proof. The trees $T_n$ have the same number of vertices $n$, and pendent vertices $p$, then we have:

\[
T_{n_i} = T_{n_j} = T_n
\]
\[
p_i = p_j = p
\]
\[
tw(S_1, T_{n_1}) = tw(S_i, T_{n_i}) = tw(S_1, T_n)
\]
\[
d(S_1, S_2) = d(S_i, S_{i+1})
\]

We apply (11) in the formula (7) and (8), then we get the result presented in Equation(9) and (10). 

\[11\]

III.3 Applications

In this section we present some examples of composed trees.

**Lemma 2.** Let $S_n$ a Star of order $n$. The Terminal Wiener of the Star $S_n$ is defined in [6] as:

\[
TW(S_n) = (n - 1)(n - 2)
\]

We define the Terminal Wiener of a pendent vertex $v$ in the Star $S_n$ as:

\[
tw(v, S_n) = 2(n - 2)
\]

**Proof.** By calculation.

![Diagram](image)

Figure 3: Star-Tree $T_N$ composed of $N$ Star $S_n$.

**Theorem 4.** Let $T_N$ a Star-Tree composed of the same $N$ Star $S_n$, connected by a pendent vertex $v$, (see Figure 3). The Terminal Wiener index of the tree $T_N$ is computed as:

\[
TW(T_N) = N(2N - 1)(n - 2)(n - 1) - 2N
\]
Proof. By applying Lemma 2 and the Corollary 1

**Definition 1.** The binomial tree $T_{B_k}$, is an ordered tree defined recursively in the following way, (see Figure 4):

- The binomial tree $T_{B_0}$ consists of a single vertex.

- For $k \geq 1$, the binomial tree $T_{B_k}$ is constructed from two binomial trees $T_{B_{k-1}}$, by attaching an edge which connects their roots $S$ and $S'$.

![Binomial Tree](image)

Figure 4: Binomial Tree. (note: $T_{B_{k-1}} = T'_{B_{k-1}}$).

**Theorem 5.** Let $T_{B_k}$ a binomial tree with $2^k$ vertices. Then the Terminal Wiener index $TW(T_{B_k})$ is given by:

$$TW(T_{B_k}) = k2^{2k-3} - 2^{k-2} \quad \forall k \geq 2 \quad (15)$$

Proof. Let $tw(S, T'_{B_{k-1}})$ be the distance between the root $S$ and the pendent vertices of $T'_{B_{k-1}}$, for simplicity we note $tw(S, T'_{B_{k-1}}) = tw(k)$, then we have:

$$tw(k) = 2^{k-2} + tw(k - 1) + tw(k - 2) + ... + tw(1)$$

$$tw(k - 1) = 2^{k-3} + tw(k - 2) + tw(k - 3) + ... + tw(1)$$

Then:

$$tw(k) = 2^{k-3} + 2tw(k - 1)$$

$$= (k + 2)2^{k-3}$$

We get:

$$tw(S, T_{B_{k-1}}) = tw(S', T'_{B_{k-1}}) = tw(k) - 2^{k-2} = k2^{k-3} \quad (16)$$

By applying Lemma 1 (Equation 5), and Equation 16 we get:

$$TW(T_{B_k}) = 2TW(T_{B_{k-1}}) + 2^{2k-4}(k + 1) \quad \text{for } k \geq 3 \quad (17)$$

And for $k = 2$:

$$TW(T_{B_2}) = 2TW(T_{B_1}) + 2^3 = 2^3 + 2^3 = 4^3$$
\[ TW(T_{B_2}) = 2^2 - 1 = 3 \]

Which then yield Equation 15.

\[ \text{Theorem 6. Let } T_N \text{ a Path-Tree composed of the same } N \text{ Star } S_n \text{ of order } n, \text{ The trees } S_n \text{ are connected by a set of edges } \{v_i, v_{i+1}\}. \]

- If \( v_i \in V(S_n) \), (see Figure 5 (a)), the Terminal Wiener index of the Tree \( T_N \) is computed as:

\[ TW(T_N) = N(n-1)(n-2) + N(n-1)^2 \left[ \frac{N^2 + 6N - 7}{6} \right] \quad (18) \]

- If \( v_i \in V_p(S_n) \), (see Figure 5 (b)), the Terminal Wiener index of the Tree \( T_N \) is computed as:

\[ TW(T_N) = N(n-2)(n-3) + N(n-2)^2 \left[ \frac{N^2 + 12N - 13}{6} \right] \quad (19) \]

\[ \text{Proof. By applying Lemma 2 and the Corollary 2.} \]

\[ \text{Figure 5: Path-Tree composed of the same } N \text{ Star } S_n. \]

\section*{IV Conclusion}

In this article we have given formulas to calculate the Terminal Wiener of composed trees connected by a pendent vertex \( S \) (Star-Tree), and those connected by a set of edges \( \{S_i, S_{i+1}\} \) (Path-Tree). We have finished our work by presenting some examples for the Star-Tree and Path-Tree composed of the same \( N \) trees, as the Star \( S_n \), and the Binomial Tree \( T_{B_k} \).
References


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