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HYPER-WIENER AND SCHULTZ INDICES OF GENERALIZED BE THE TREES

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Abstract

Let G be a simple, undirected and connected graph. The Schultz molecular topological index of G, denoted by $MTI(G)$, is defined to be the summation $MTI(G) = \sum_{i,j} \deg(i)(d(i, j) + A(i, j))$, where $\deg(i)$ is the degree of vertex i in G, $d_G(i, j)$ is the distance between vertices i and j and $A(i, j)$ is the (i, j)-th entry of the adjacency matrix A of G. The hyper-Wiener index of a chemical tree T is defined as the sum of the products $n_1 n_2$, over all pairs u, v of vertices of T, where n_1 and n_2 are the number of vertices of T, lying on the two sides of the path which connects u and v. In this paper we compute the hyper-Wiener index and Schultz index of generalized Bethe trees. In special case these topological indices will be computed for dendrimer and regular starlike trees.

1. Introduction

A topological index of a graph is a real number related to structure of the molecular graph. It does not depend on the labelling or pictorial representation of the graph. In 1947, Harold Wiener [11] developed the most widely known topological descriptor, the Wiener index, and used it to determine physical properties of types of alkanes known as paraffin. Let T be a tree (i.e., a connected and acyclic graph). Let e be an edge of T, joining the (adjacent) vertices u and v. Denote by $n_u(e)$ the number of vertices of T lying on one side of the edge e, closer to vertex u. Denote by $n_v(e)$ the number of

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vertices of T lying on the other side of the edge e, closer to vertex v. (Because T is acyclic, the quantities $n_u(e)$ and $n_v(e)$ are unambiguously determined for every edge.) Then the Wiener index of T is defined as

$$W(T) = \sum_{e} n_u(e)n_v(e), \tag{1}$$

in which the summation goes over all edges of T. The hyper-Wiener index is a graph invariant, put forward by Randić as a kind of extension of the Wiener index [8]. Let T be a tree and u, v be arbitrary pair of vertices of T. These vertices are joined by a unique path which we denote by p. Denote by $n_u(p)$ the number of vertices of T lying on one side of the path p, closer to vertex u. Denote by $n_v(p)$ the number of vertices of T lying on the other side of the path p, closer to vertex v. (Again, because T is acyclic, the quantities $n_u(p)$ and $n_v(p)$ are unambiguously determined for every path.) Then the hyper-Wiener index of T is defined as

$$WW(T) = \sum_{p} n_u(p)n_v(p), \tag{2}$$

in which the summation goes over all paths of T.

The Schultz index of a molecular graph G was introduced by Schultz [9] in 1989 for characterizing alkanes by an integer as follows:

$$MTI(G) = \sum_{i,\, j} \deg(i)(d(i,\, j) + A(i,\, j)), \tag{3}$$

where $\deg(i)$ is vertex degree of i, $d(i, j)$ is the distance between i and j and $A(i, j)$ is the (i, j) entry of the adjacency matrix of G. The Schultz index has been shown to be a useful molecular descriptor in the design of molecules with desired properties [3]-[7].

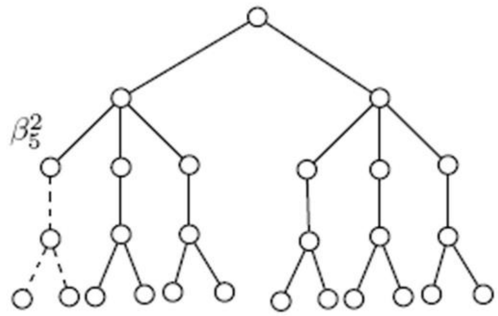

Figure 1. A generalized Bethe tree of 5 levels and its subtree β_5^2.

A generalized Bethe tree β_k is an unweighted rooted tree with k levels such that in each level the vertices have equal degree. For example factorial trees, dendrimer trees and starlike trees in which all of the pendent vertices have equal distances from central vertex (regular starlike trees) can be considered as generalized Bethe tree. If all the non-pendent vertices of a tree have equal degree, then the tree is called dendrimer tree. Denote by $D_{p,r}$ the dendrimer tree with $r+1$ levels in which degree of non-pendent vertices is $p+1$. In the last few years calculation of topological indices of the generalized Bethe trees has been a research topic in chemical graph theory [1]-[2]. In this paper we compute the hyper-Wiener index and Schultz index of generalized Bethe tree in term of number of levels and degrees of vertices of the tree. As application of introduced methods the hyper-Wiener and Schultz index of dendrimer and regular starlike trees will be calculated.

2. Hyper-Wiener Index

In this section the hyper-Wiener index of generalized Bethe trees with $k+1$ levels will be computed by using Equation (2). Throughout the paper we suppose that the rooted vertex of β_{k+1} is located on level 0 and pendent vertices are located on level k. Denote by d_i the degree of vertices on the level i, for $i = 0, 1, 2, \ldots, k$. Put

$$e_i = \begin{cases} d_i & \text{if} \quad i = 0 \\ d_i - 1 & \text{if} \quad i \neq 0. \end{cases}$$

Therefore if n_i denotes the number of vertices on the level i, then $n_0 = 1$ and $n_i = \prod_{j=0}^{i-1} e_j$ for $i = 1, 2, 3, \ldots, k$. If v is one of the n_i vertices on the level i for $0 \le i \le k$, the number of vertices of β_{k+1}^{i}, the subtree of β_{k+1} where v can be considered as its rooted vertex (see Figure 1) is computed as follows:

$$N_i = 1 + \sum_{j=i}^{k} n_j.$$

Let u be a vertex on the level i and v be a vertex on the level j of β_{k+1} for $0 \le i \le j \le k$. Denote by $p_{i,j}$ the unique path of β_{k+1} joining the vertices u and v. By using symmetry of the graph, the values of $n_u(p_{i,j})$ and $n_v(p_{j,i})$ are equal. In continue the hyper-Wiener index of generalized Bethe tree will be computed by considering of this point.

Theorem 1. *Let β_{k+1} be a generalized Bethe tree with $k+1$ levels. Then the hyper-Wiener index of β_{k+1} is computed as*

$$WW = \sum_{j=1}^{k} n_j N_j (N_0 - N_1) + \sum_{i=1}^{k} \binom{n_i}{2} N_i^2$$
$$+ \sum_{i=1}^{k-1} n_i \sum_{j=i+1}^{k} [N_i N_j (n_i - \prod_{r=i+1}^{j} e_r) + (N_0 - N_{i+1}) N_j \sum_{r=i+1}^{j} e_r].$$

Proof. Let $p_{0,j}$ denote the unique path of β_{k+1} joining v, the root vertex of the graph, and u, a vertex on the level j of the graph. Then $n_v(p_{0,j}) = N_j$ and $n_u(p_{0,j}) = N_0 - N_1$ for $1 \le j \le k$. Now let $p_{i,i}$ denote the unique path joining two vertices u and v on the level i, then $n_u(p_{i,i}) = n_v(p_{i,i}) = N_i$ for $1 \le i \le k$. At last suppose that $p_{i,j}$ denotes the unique path joining vertices u on the level i and v on the level j of β_{k+1} for $0 \le i < j \le k$. Then for $\prod_{r=i+1}^{j} e_r$ vertices on the level j such that u is their common parent, we have $n_u(p_{i,j}) = N_0 - N_{i+1}$ and $n_v(p_{i,j}) = N_j$. For the other vertices on the level j we have $n_u(p_{i,j}) = N_i$ and $n_v(p_{i,j}) = N_j$. Thus by using Equation (2) the hyper-Wiener index of β_{k+1} is computed as follows:

$$\begin{aligned}
WW &= \sum_p n_u(p)n_v(p) \\
&= \sum_{j=1}^{k} n_j[n_u(p_{0,j})n_v(p_{0,j})] + \sum_{i=1}^{k}\binom{n_i}{2} n_u(p_{i,i})n_v(p_{i,i}) \\
&\quad + \sum_{i=1}^{k-1}\sum_{j=i+1}^{k} n_i n_j[n_u(p_{i,j})n_v(p_{i,j})] \\
&= \sum_{j=1}^{k} n_j N_j(N_0 - N_1) + \sum_{i=1}^{k}\binom{n_i}{2} N_i^2 \\
&\quad + \sum_{i=1}^{k-1} n_i \sum_{j=i+1}^{k} [(n_i - \prod_{r=i+1}^{j} e_r)N_i N_j + \prod_{r=i+1}^{j} e_r(N_0 - N_{i+1})N_j].
\end{aligned}$$

Therefore theorem is proved. □

In order to introduce some applications of Theorem 1 we will compute the hyper-Wiener index of some molecular graphs.

Dendrimers are hyperbranched molecules, synthesized by repeatable steps, either by adding branching blocks around a central core or by building large branched blocks starting from the periphery and then attaching them to the core (the "convergent growth" approach [4]). The vertices of a dendrimer, except the external end points, are considered as branching points. The number of edges emerging from each branching point is called progressive degree, (i.e., the edges which enlarge the number of points of a newly added orbit). A regular dendrimer, of progressive degree p and generation r is herein denoted by $D_{p,r}$ (see Figure 2).

The hyper Wiener of dendrimer trees was calculated by Diudea and Prav [4]. In continue we obtain their result by using Theorem 1 and compute the hyper-Wiener index of $D_{p,r}$ in terms of positive integers p and r.

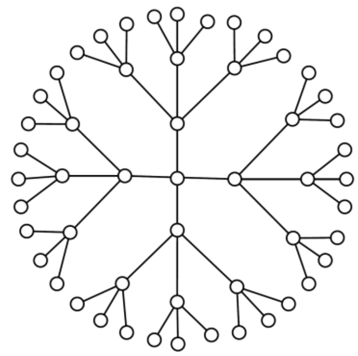

Figure 2: The graph of $D_{3,3}$.

Corollary 1. *Let $D_{p,r}$ be a dendrimer tree with $r+1$ levels which degree of its non-pendent vertices is equal to $p+1$. The hyper-Wiener index of $D_{p,r}$ is given as*

$$WW(D_{p,r}) = \frac{1}{2(p-1)^4}(2p^{2r}(p^2-1)r^2 + p^{2r}(p^2-1)(p^2-8p-5)r$$

$$+(p+1)(p^r-1)[p^r(p^2-10p+3)-2]).$$

Proof. Since $D_{p,r}$ is a generalized Bethe tree with $r+1$ levels such that $e_0 = p+1$ and $e_i = p$ for $1 \le i \le r-1$, hence $n_0 = 1$ and $n_i = (p+1)p^{i-1}$ for $1 \le i \le r$. Therefore

$$N_i = \sum_{j=0}^{r-i} p^j = \frac{(p^{r-i+1}-1)}{p-1},$$

for $1 \le i \le r$ and $N_0 = (p+1)p^{r-1}$. The results can be obtained by replacing value of n_i and N_i for $0 \le i \le r$ in the obtained formula in Theorem 1. □

In the following corollary we consider a starlike tree where the distances between its pendent vertices is equal (regular starlike tree). Denote by $T_{p,r}$ this starlike tree if the vertex degree of its central vertex is p and distance between the pendent vertices and central vertex is r. The hyper-Wiener index of $T_{p,r}$ can be computed by using Theorem 1 as follows.

Corollary 2. *The hyper-Wiener index of starlike tree* $T_{p,r}$ *is computed as*

$$WW(T_{p,r}) = \frac{p^2r^2}{24}(7r^2 + 18r + 11) - \frac{pr}{4}(r^3 + 2r^2 - 1).$$

Proof. Since $T_{p,r}$ can be considered as a generalized Bethe tree of $r+1$ levels such that $e_0 = p$ and $e_i = 2$ for $1 \leq i \leq r-1$, hence $n_0 = 1$, $N_0 = rp + 1$, $n_i = p$ and $N_i = r - i + 1$ for $1 \leq i \leq r$. Therefore by using Theorem 1 we have

$$WW(T_{p,r}) = \sum_{i=1}^{r} p(r-i+1)(rp+1-r) + \sum_{i=1}^{r} \frac{p(p-1)}{2}(r-i+1)^2$$

$$+ \sum_{i=1}^{r-1} p \sum_{j=i+1}^{r} ((r-i+1)(r-j+1)(p-1) + (rp+1-(r-j))(r-j+1))$$

$$= \frac{p^2r^2}{24}(7r^2 + 18r + 11) - \frac{pr}{4}(r^3 + 2r^2 - 1).$$

Therefore corollary is proved.

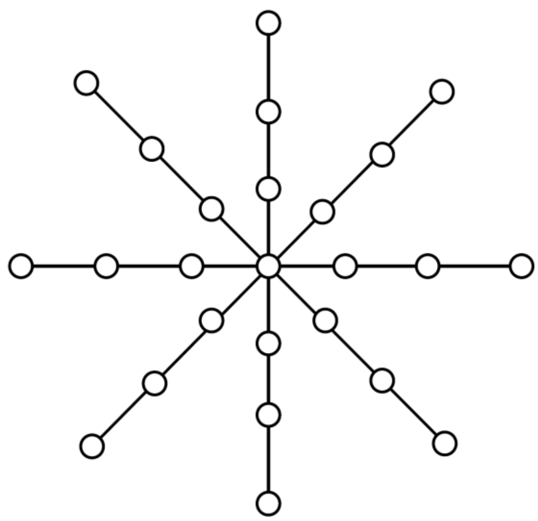

Figure 3. A regular starlike tree, $T_{8,3}$.

3. Schultz Index

In this section the Schultz index of β_{k+1} will be computed by using the obtained results in previous section. By consideration Equation (3), the sum of the distances between an arbitrary vertex and all of the other vertices of the graph must be computed. For this purpose we will use a method similar to what is used in calculation the Wiener index of a graph (see Equation (1)).

Let v_0 be an arbitrary vertex and $e = uv$ be an arbitrary edge of the simple graph G. If v_0 is closer to vertex u than vertex v, put $n_u^*(e) = 1$ and $n_v^*(e) = n_v(e)$. The sum of the distances between v_0 and all of the other vertices of G is computed as follows:

$$S(v_0) = \sum_{e \in E(G)} n_u^*(e) n_v^*(e) = \sum_{e \in E(G)} n_v(e). \tag{4}$$

In the following theorem the Schultz index of β_{k+1} is computed by using Equations (3) and (4).

Theorem 2. *Let $k > 1$ be an positive integer. Then the Schultz index of the generalized Bethe tree with $k+1$ levels is computed as*

$$MTI(\beta_{k+1}) = \sum_{i=0}^{k} \left(n_i d_i \left(\sum_{j=1}^{i} [N_0 + (n_{i-j+1} - 2) N_{i-j+1}] + \sum_{j=i+1}^{k} n_j N_j \right) + d_i^2 \right).$$

Proof. Let x_i be one of the vertices on level i of β_{k+1} for $0 \leq i \leq k$. In order to computation the sum of the distances between x_i and all of the other vertices of the graph assume that $e = uv$ adjacent two vertices on the levels j and $j+1$ of the graph. If $j \geq i$, then

$$n_v(e) = \sum_{j=i+1}^{k} n_j N_j.$$

Now suppose that $j < i$, we have

$$n_v(e) = \sum_{j=1}^{i} (N_0 + (n_{i-j+1} - 2) N_{i-j+1}).$$

At last by using Equations (3) and (4) the Schultz index of β_{k+1} is computed as follows:

$$MTI(\beta_{k+1}) = \sum_{i=0}^{k} d_i (n_i S(x_i) + d_i)$$

$$= \sum_{i=0}^{k} \left(n_i d_i \left(\sum_{j=1}^{i} [N_0 + (n_{i-j+1} - 2) N_{i-j+1}] + \sum_{j=i+1}^{k} n_j N_j \right) + d_i^2 \right).$$

Therefore theorem is proved. □

In continue, as application of Theorem 2 the Schultz index of dendrimer trees and regular starlike trees will be computed.

Corollary 3. *Let $D_{p,r}$ be a dendrimer tree with $r+1$ levels such that degree of its non-pendent vertices is $p+1$. The Schultz index of $D_{p,r}$ is given as*

$$MTI(D_{p,r}) = \frac{1}{p(p-1)^3} (p^{2r+1}[p^3(4r-1) + p^2(4r-9) - p(4r+11) - 4r - 3]$$

$$+ p^{r+1}[p^4 + 3p^3 + 7p^2 + 13p + 8] - p(2p^4 - 2p^2 + 4p + 4)).$$

Proof. Let $e_0 = p+1$ and $e_i = p$ for $1 \leq i \leq r-1$. Thus $n_0 = 1$, $n_i = (p+1)p^{i-1}$ and $N_i = \dfrac{p^{r-i+1} - 1}{p-1}$ for $1 \leq i \leq r$. Therefore by using Equation (3) we have

$$S(x_i) = \sum_{j=1}^{i} [N_0 + (n_{i-j+1} - 2) N_{i-j+1}] + \sum_{j=i+1}^{r} n_j N_j$$

$$= \frac{p^r [p^3(r+i) + p^2(2p^{-i} - 3) - p(r+i+1)] + p(p+1)}{p(p-1)^2}. \qquad (5)$$

Since $\deg(v) = p+1$, if v is a non-pendent vertex and $\deg(v) = 1$ for pendent vertices of the graph, by using Equation (3)

$$MTI(D_{p,r}) = \sum_{i=0}^{r-1} [n_i(p+1)(S(x_i) + p + 1)] + n_r(S(x_r) + 1).$$

The result is obtained by replacing Equation (4) in the last equation. □

Corollary 4. *Let $T_{p,r}$ be a regular starlike tree with $r+1$ levels in which degree of its rooted vertex is p. Then*

$$MTI(T_{p,r}) = p^2(2r^3 + r^2 + 1) - \frac{p}{3}(4r^3 - 13r + 9).$$

Proof. Let $e_0 = p$ and $e_i = 2$ for $1 \le i \le r-1$. So $n_0 = 1, N_0 = rp+1, n_i = p$ and $N_i = r - i + 1$ for $1 \le i \le r$. By using Equation (3) we have

$$S(x_i) = \sum_{j=1}^{i} [pr + 1 + (p-2)(r-j+1)]$$

$$+ \sum_{j=i+1}^{r} p(r-j+1) = \frac{p}{2}(r^2 + r + 2ri) - i(2r - i).$$

Since for rooted vertex of the graph vertex degree is p, for other non-pendent vertices vertex degree is 2 and for pendent vertices of the graph vertex degree is 1, so

$$MTI(T_{p,r}) = p(S(x_0) + p) + \sum_{i=1}^{r-1} 2p(S(x_i) + 2) + p(S(x_r) + 1).$$

The result is obtained by replacing (4) in the last equation. □

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