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The Hosoya-Wiener Polynomial of Weighted Trees

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Formulas for the Wiener number and the Hosoya-Wiener polynomial of edge and vertex weighted graphs are given in terms of edge and path contributions. For a rooted tree, the Hosoya-Wiener polynomial is expressed as a sum of vertex contributions. Finally, a recursive formula for computing the Hosoya-Wiener polynomial of a weighted tree is given.

INTRODUCTION

In this paper we consider the vertex and edge weighted graphs where the weights are positive real numbers. In mathematical chemisty, molecules are often modelled by graphs. The sum of all distances is known as the Wiener number.[1] It was the first non-trivial topological index in chemistry, which was introduced by H. Wiener in 1947 to study boiling points of paraffins (for historical data, see for instance Ref. 2). Since then, the Wiener number (also called the Wiener index) has been used to explain various chemical and physical properties of molecules and to correlate the structure of molecules with their biological activity. The research interest in the Wiener number and related indices is still considerable.[3,4]

The Hosoya-Wiener polynomial of a graph G is defined as:

$$W(x) = W(\mathrm{G};\, x) = \sum x^{d(u,v)}, \tag{1}$$

where the sum runs over all unordered pairs of vertices $u,\ v \in V\,(\mathrm{G})$. This definition, which is used for example in Ref. 5, slightly differs from the definition used by Hosoya[6] (see also Ref. 7):

$$\hat{W}(x) = \hat{W}(\mathrm{G};x) = \sum_{u \neq v} x^{d(u,v)}. \tag{2}$$

Obviously, $W(x) = \hat{W}(x) + |V(\mathrm{G})|$.

In his paper[6] Hosoya used the name Wiener polynomial while some authors later used the name Hosoya polynomial.[8,9] We decided to use a compromise name here, namely the Hosoya-Wiener polynomial.

It is well known that the first derivative of the Hosoya-Wiener polynomial evaluated at $x = 1$ equals the Wiener number (see for example Ref. 7). Higher derivatives of the Hosoya-Wiener polynomial have also been used as descriptors.[10,11]

In an arbitrary tree, every edge is a bridge, *i.e.*, after deletion of an edge, the graph is no more connected. The contribution to the Wiener number of an edge was taken to be the product of the numbers of vertices in the two connected components. This number also equals the num-

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ber of all shortest paths in the tree that go through the edge.[12] Therefore the usual generalization of the Wiener number on arbitrary graphs is defined to be the sum of all distances in a graph. Recalling and generalizing the original definition, edge contributions to the Wiener number were studied in Refs. 13, 14, 15. Here we study edge and path contributions to the Hosoya-Wiener polynomial of weighted graphs.

We claim that the algorithm given in Ref. 16 can be generalized to compute the Hosoya-Wiener polynomial. However, not only the sum of all distances, but the distance distribution is nedeed for the polynomial. Hence, a vector of distances has to be mantained and the complexity of computation will necessarily include an additional factor related to the number of different distances that appear in the graph. Here we discuss a generalization of trees and give a recursive formula for the Hosoya-Wiener polynomial of a rooted tree.

PRELIMINARIES

A weighted graph G = G(V,E,ω,λ) is a combinatorial object consisting of an arbitrary set $V = V$ (G) of vertices, a set $E = E$(G) of unordered pairs $\{x, y\} = xy$ of distinct vertices of G called edges, and two weighting functions, w and λ. $w : V(\mathrm{G}) \mapsto \mathrm{IR}^+$ assigns positive real numbers (weights) to vertices and $\lambda : E(\mathrm{G}) \mapsto \mathrm{IR}^+$ assigns positive real numbers (lengths) to edges. Without a loss of generality, we will assume $V(\mathrm{G}) = \{1, 2, 3, ..., n\}$.

A simple path from u to v is a finite sequence of distinct vertices $P = x_0, x_1, ..., x_l$ such that each pair x_{i-1}, x_i is connected by an edge and $x_0 = u$ and $x_l = v$. The length of the path is the sum of the lengths of its edges, $l(P) = \sum_{i=1}^{l} \lambda(x_{i-1}\, x_i)$. For any pair of vertices u, v, we define the distance $d(u, v)$ to be the minimum of lengths over all paths between u and v. If there is no such path, we write $d(u, v) = \infty$.

A graph G is connected if $d(x, y) < \infty$ for any pair of vertices x, y. A tree is a connected graph with $|E(G)| = |V(G)| - 1$. A rooted tree is just a tree in which one vertex is called the root. For the usual graph theoretical terminology not defined here see, for instance, Ref. 17.

HOSOYA-WIENER POLYNOMIAL

The Hosoya-Wiener polynomial of a weighted graph G is defined as:

$$W(x) = W(\mathrm{G},\ \lambda,\ w;\ x) = \sum_{u \le v} w(u)w(v)x^{d(u,v)}. \qquad (3)$$

Recently, Klein, Došlić and Bonchev[18] generalized the Hosoya-Wiener polynomial to vertex weighted graphs in two ways that slightly differ from the one given here.

Clearly, our definition is equivalent to the original definition (1) if all vertex and edge weights are equal to 1. Note that in this case we get $W(\mathrm{G}, 1, 1; x) = W(x) = \sum_{u,v \in V(\mathrm{G})} x^{d(u,v)}$ like in Ref. 5.

Remark. The generalization $W(\mathrm{G}, \lambda, w; x)$ studied here may not be a polynomial if the edge weights are allowed to be arbitrary real numbers. Obviously, if natural numbers are used for edge weights, the function $W(\mathrm{G}, \lambda, w; x)$ is a polynomial. Hence, with appropriate scaling factor, one can always consider $W(\mathrm{G}, \lambda, w; x)$ to be a polynomial, for any model using rational edge weights.

The weighted Wiener number[19] of a weighted graph G is:

$$W = W(\mathrm{G},\ \lambda,\ w) =$$

$$\sum_{u<v} w(u)w(v)d(u,v) = \sum_{u \le v} w(u)w(v)d(u,v)\,. \qquad (4)$$

This definition is clearly a generalization of the usual definition of the (unweighted) Wiener number. More precisely, if all weights of vertices are 1 and all lengths of edges are 1, then $W(\mathrm{G}, \lambda, w)$ is the usual Wiener number $W(\mathrm{G})$.

It seems that the weighted Wiener number has not been studied frequently in the literature. In Ref. 19, a linear algorithm for computing the weighted Wiener number is given. A definition, analogous to (4), was used in Refs. 20 and 21 for vertex weighted graphs. A different definition, in which the »weights« of atoms are added to the sum of distances, is given in Ref. 22. Weight distances with the reverse of bond order are used in Ref. 23. Let us just mention perhaps the most interesting property of the Hosoya-Wiener polynomial, namely $W'(\mathrm{G}, \lambda, w; x) = W(\mathrm{G}, \lambda, w)$.

A REMARK ON EDGE AND PATH CONTRIBUTIONS

We first show how the weighted Wiener number of a general weighted graph can be seen as a sum of path and edge contributions.

Lemma 1. – For a weighted graph $\mathrm{G} = \mathrm{G}(V, E, w, \lambda)$,

$$W(\mathrm{G}) = \sum_{e=uv} \lambda(e) \cdot \sum_{P^*_{a,b} \ni e} \frac{1}{n^*(a,b)} w(a)w(b)\,,$$

where $P^*_{a,b}$ is a shortest path between a and b and $n^*(a; b)$ is the number of shortest paths with endpoints a and b.

Proof. To see this, it is enough to sum up the contributions of each edge to $W(\mathrm{G})$ in two different ways. Each pair a, b of vertices contributes $w(a)w(b)d(a, b)$ to the Wiener number. This contribution can be either regarded as a contribution of the pair a, b or it can be divided into

$n^*(a, b)$ path contributions, which can be further regarded as a sum of edge contributions along the path. Since $d(a, b)$ is the sum of edge weights along a shortest path, the contribution of edge:

$$\lambda(e) \frac{1}{n^*(a,b)} w(a)w(b) .$$

An edge contributes as many times as it appears on various shortest paths. Here the vertices are weighted, so one has to take into account the weights of both terminal vertices. Let us note in passing that the sum of contributions of the edge e:

$$\omega^*(e) := \sum_{P^*_{a,b} \ni e} \frac{1}{n^*(a,b)} w(a)w(b) ,$$

can be called the shortest path weight distribution, generalizing the ideas of Refs. 13, 14, 15.

Hence, one can sum up the lengths of all shortest paths (like in (4)), or, equivalently, sum up the contributions of all edges.

Recall that on a tree, there is a unique shortest path between any pair of vertices. Hence $n^*(a, b) = 1$ for all a, b.

From Lemma 1 we read that the path contribution of a shortest path $P = P^*_{a,b}$ between vertices a and b is:

$$\frac{1}{n^*(a,b)} w(a)w(b) \sum_{e \in P^*_{a,b}} \lambda(e) ,$$

and the contribution of an edge e is:

$$\lambda(e) \cdot \sum_{P^*_{a,b} \ni e} \frac{1}{n^*(a,b)} w(a)w(b) .$$

Note that the path contribution can be seen as a sum of (partial) edge contributions related to the path and the edge contribution can be seen as a sum of path contributions related to the edge.

However, the next lemma shows that for the Hosoya-Wiener polynomial, the path contributions can again be seen as sums of (partial) edge contributions related to the path, but the situation is slightly different for the edge contributions.

Lemma 2. – For a weighted graph G,

$$W(\mathrm{G}, \lambda, w; x) = \sum_{a<b} \sum_{P^*_{a,b}} \frac{1}{n^*(a,b)} w(a)w(b) \prod_{e \in P^*_{a,b}} x^{\lambda(e)},$$

where $P^*_{a,b}$ is a shortest path between a and b and $n^*(a; b)$ is the number of shortest paths with endpoints a and b.

Proof. To see this, it is enough to sum up the contributions of each edge to $H(\mathrm{G}; \lambda, w; x)$ in two different ways. Each pair a, b of vertices contributes $w(a)w(b)x^d(a, b)$ to the Hosoya-Wiener polynomial. This contribution can be either regarded as a contribution of the pair a, b or it can be divided into $n^*(a, b)$ path contributions:

$$x^{d(a,b)} \frac{1}{n^*(a,b)} w(a)w(b) ,$$

which can be further regarded as a product of edge contributions along the path.

$$x^{d(a,b)} \frac{1}{n^*(a,b)} w(a)w(b) = \frac{1}{n^*(a,b)} w(a)w(b) \prod_{e \in P^*_{a,b}} x^{\lambda} (e) .$$

Hence, one can sum up the contributions of all shortest paths, but note that the edge contributions to the path contribution are multiplied, and not added. Representing the Hosoya-Wiener in terms of edge contributions is hence somewhat more complicated in the following sense. For each path crossing the edge, one needs to know the amount of traffic (in a possible natural model, the intensity of the traffic corresponds to $\frac{1}{n^*(a,b)} w(a)w(b)$, *i.e.*, the number of packets between a and b that use the path through e), but also the length of the paths. Edge contribution can be given by:

$$w(e) = \sum_{P^*_{a,b} \ni e} x^{d(a,b)} \frac{1}{n^*(a,b)} w(a)w(b),$$

where, obviously, besides the amount of traffic some information on the source and sink of the traffic is taken into account.

HOSOYA-WIENER POLYNOMIAL ON TREES

Assume we are given a rooted tree T. For each vertex $v \in \mathrm{T}$, let $W_{\bar{v}}(x)$ denote the partial Hosoya-Wiener polynomial corresponding to all distances from v to all other vertices in the subtree, rooted at v. By definition $W_{\bar{v}}(x) = 0$, if v is a leaf.

Lemma 3. – Let $v_1, v_2, ..., v_k$ be the sons of a vertex v in a rooted tree T with partial Hosoya-Wiener polynomials $W_{\bar{v}_1}(x), W_{\bar{v}_2}(x), \ldots, W_{\bar{v}_k}(x)$, respectively. Then, the partial Hosoya-Wiener polynomial at vertex v can be computed as follows:

$$W_{\bar{v}}(x) = w(v) \sum_{i=1}^{k} \left(\frac{W_{\bar{v}_1}(x)}{w(v_i)} + w(v_i) \right) x^{\lambda(v_i v)}$$

Proof. The path from v to v_i contributes $w(v_i)x^{\lambda(v_i v)}w(v)$. The contribution of the path from v to w in the subtree, rooted at v_i, can be written as:

$$w(w)x^{d(w,v)}w(v) = w(w)x^{d(w,v_i)+\lambda(v_i v)}w(v) =$$

$$w(w)x^{d(w,v_i)}x^{\lambda(v_i v)}w(v) =$$

$$w(w)x^{d(w,v_i)}w(v_i)\frac{1}{w(v_i)}x^{\lambda(v_i v)}w(v)$$

Hence, the sum over all vertices w from the subtree rooted at v_i and the sum over all sons v_i of v gives the result claimed:

$$W_{\vec{v}}(x) = w(v)\sum_{w\in T_v} x^{d(w,v)}w(w) =$$

$$w(v)\sum_{w\in T_v} w(w)\sum_{i=1}^{k} x^{d(w,v_i)}w(v_i)\frac{1}{w(v_i)}x^{\lambda(v_i v)} =$$

$$w(v)\sum_{i=1}^{k}\frac{1}{w(v_i)}x^{\lambda(v_i v)}\sum_{w\in T_{v_i}} w(w)x^{d(w,v_i)}w(v_i) =$$

$$w(v)\sum_{i=1}^{k}\frac{1}{w(v_i)}x^{\lambda(v_i v)}(W_{\vec{v}_i}(x) + w(v_i)^2) =$$

$$w(v)\sum_{i=1}^{k}\left(\frac{W_{\vec{v}_i}(x)}{w(v_i)} + w(v_i)\right)x^{\lambda(v_i v)}.$$

For each vertex $v \in$ T, let $W_v(x)$ denote the contribution of the vertex v to the Hosoya-Wiener polynomial. This contribution corresponds to all shortest paths in the subtree, rooted at vertex v, which meet v.

On the other hand, each path P in a rooted tree meets a unique vertex v at a minimal distance from the root. The contribution of the path P is thus counted in the $W_v(x)$, and at no other vertex. Furthermore note that each path meets at least one vertex that is not a leaf.

Lemma 4. – Let $v_1, v_2, ..., v_k$ be the sons of a vertex v in a rooted tree T with partial Hosoya-Wiener polynomials $W_{\vec{v}_1}(x), W_{\vec{v}_2}(x), \ldots, W_{\vec{v}_k}(x)$, respectively. Then, the contribution $W_v(x)$ of the vertex v to the Hosoya-Wiener polynomial is:

$$W_v(x) = \frac{1}{2}\left[\left(\frac{1}{w(v)}W_{\vec{v}}(x) + w(v)\right)^2 + \sum_{i=1}^{k}\left(\frac{1}{w(v_i)}W_{\vec{v}_i}(x) + w(v_i)\right) \cdot x^{\lambda(v_i v)} - \sum_{i=1}^{k}\left(\left(\frac{1}{w(v_i)}W_{\vec{v}_i}(x) + w(v_i)\right)\cdot x^{\lambda(v_i v)}\right)^2 + w(v)^2\right]$$

Proof. Any shortest path that meets vertex v consists of one or can be built from two shortest paths from v (*i.e.*, either a path of the form v ... x or a concatenation of two paths of the form x ... v ... y).

The contribution of vertex v to the Hosoya-Wiener polynomial is therefore the sum of:

$$x^{\lambda(v_i v)}\frac{w(v)}{w(v_i)}W_{\vec{v}_i}(x)$$

for all neighbors v_i of v and

$$x^{\lambda(v_i v)}x^{\lambda(v_j v)}\frac{1}{w(v_i)w(v_j)}W_{\vec{v}_i}(x)W_{\vec{v}_j}(x)$$

over all pairs of neighbors of v. For brevity, let us denote:

$$C_i = \left(\frac{1}{w(v_i)}W_{\vec{v}_i}(x) + w(v_i)\right)\cdot x^{\lambda(v_i v)}.$$

Note that Lemma 3 in new notation reads $W_{\vec{v}}(x) = w(v)\cdot\sum_{i=1}^{k} C_i$. Obviously,

$$\left(\frac{1}{w(v)}W_{\vec{v}}(x) + w(v)\right)^2 = \left(w(v) + \sum_{i=1}^{k} C_i\right)^2 =$$

$$w(v)^2 + w(v)\sum_{i=1}^{k} C_i + \sum_{i=1}^{k}\sum_{j=1}^{k} C_i C_j =$$

$$w(v)^2 + w(v)\sum_{i=1}^{k} C_i + \sum_{i<j} C_i C_j + \sum_{i=1}^{k} C_i^2 + \sum_{i>j} C_i C_j$$

and because $\sum_{i<j} C_i C_j = \sum_{i>j} C_i C_j$, we have

$$\sum_{i<j} C_i C_j =$$

$$\frac{1}{2}\left(\left(\frac{1}{w(v)}W_{\vec{v}}(x) + w(v)\right)^2 - w(v)\sum_{i=1}^{k} C_i - \sum_{i=1}^{k} C_i^2 - w(v)^2\right).$$

The shortest paths in the subtree rooted at vertex v that meet v include paths with none, one or both endpoints equal vertex v. (The last case corresponds to a path of distance 0.) Hence:

$$W_v(x) = w(v)\sum_{i=1}^{k} C_i + \sum_{i<j} C_i C_j + w(v)^2 =$$

$$\frac{1}{2}\left(\left(\sum_{i=1}^{k} C_i + w(v)\right)^2 + w(v)\sum_{i=1}^{k} C_i - \sum_{i=1}^{k} C_i^2 + w(v)^2\right).$$

CONCLUSIONS

From the above results, a recursive formula for the Hosoya-Wiener polynomial of a tree can be deduced.

Theorem 5. – Let $v_1, v_2, ..., v_k$ be the sons of a vertex v in a rooted tree T with Hosoya-Wiener polynomials $W(T_{v_1}, w, \lambda; x)$, $W(T_{v_2}, w, \lambda; x)$, ..., $W(T_{v_k}, w, \lambda; x)$ and with partial

Hosoya-Wiener polynomials $W_{\bar{v}_1}(x), W_{\bar{v}_2}(x), \ldots, W_{\bar{v}_k}(x)$. Let T_u denote the subtree of T with root u. Then, the Hosoya-Wiener polynomial of the subtree rooted at v is:

$$W(T_v, w, \lambda; x) = \sum_{u \in V(T_v)} W_u(x) = W_v(x) + \sum_{v_i} W(T_{v_i}, w, \lambda; x)$$

Recall that $W_v(x)$ can be computed from partial polynomials of the sons of v by Lemma 3. Therefore the formula also gives a recursive algorithm:

ALGORITHM A ((T_v, v): rooted tree with root)

(i) for all sons v_i of v run A(T_{v_i}, v_i) (compute Hosoya-Wiener polynomial $W(T_{v_i}, w, \lambda; x)$ and partial Hosoya-Wiener polynomial $W_{\bar{v}_i}(x)$)

(ii) combine the results and return $W(T_v, w, \lambda; x)$ (and $W_{\bar{v}}(x)$).

Given a tree T with an arbitrary vertex r, running A(T, r) returns the Hosoya-Wiener polynomial W(T, w, λ; x). Another way of writing the algorithm without recursion is:

ALGORITHM B

(i) given a weighted tree T, choose any vertex and call it the root

(ii) order the vertices in the BFS order (breadth first search from the root)

(iii) visit the vertices in the reverse BFS order and compute the $W_{\bar{v}}(x)$

(iv) compute (in any order) $W_v(x)$ and sum up over all vertices that are not leaves. The sum equals W(T, w, λ; x).

The correctness of the two algorithms is a straightforward consequence of the results proved in the previous section. We omit the details.

Theorem 6. – The algorithms A and B give the Hosoya-Wiener polynomial on a weighted tree T.

Remark. If arbitrary edge weights are allowed, then the function $W(G, w, \lambda; x)$ is generally not a polynomial. Furthermore, one can find examples where up to $n(n-1)/2$ different values for distances appear. Hence, a simple analysis yields the complexity estimate $O(n^3)$, which is no better than the complexity of computing all distances in a weighted graph with standard algorithms (for example, p. 200 of Ref. 17). It does not seem likely that the present approach would give a competitive way of computing the Hosoya-Wiener polynomial on trees with arbitrary weights.

On the other hand, we believe that it is possible to generalize the approach outlined here to cacti, which may be an interesting avenue of further research.

Example. Given a tree, let us choose one vertex and draw the tree rooted at the vertex as shown in the Figure.

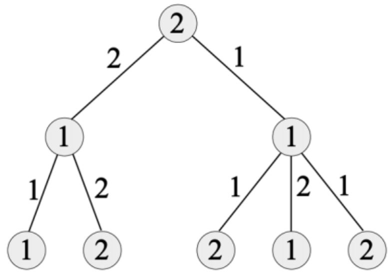


Figure 1.1. Example of weighted tree T.

Next, compute the partial Hosoya-Wiener polynomials:

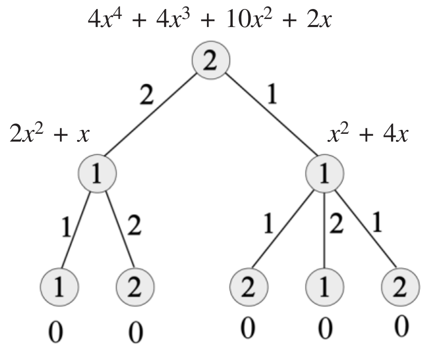
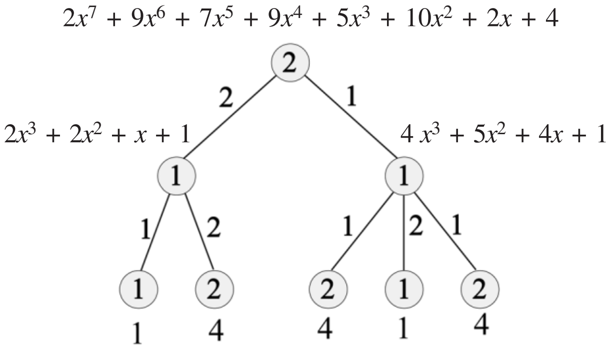


Figure 1.2. Partial Hosoya-Wiener polynomials on vertices of T.

Finally, compute the vertex contributions and their sum, giving the result.



$W(x) = 2x^7 + 9x^6 + 7x^5 + 9x^4 + 11x^3 + 17x^2 + 7x + 20$

Figure 1.3. Contribution of each vertex v to the Hosoya-Wiener polynomial $W(x)$ of T.

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SAŽETAK

Hosoya-Wienerov polinom za utežene grafove

Blaž Zmazek i Janez Žerovnik

Formule za Wienerov broj i Hosoya-Wienerov polinom grafova s uteženim čvorovima i granama izražene su pomoću doprinosa grana i puteva. U slučaju stabala s korijenom Hosoya-Wienerov polinom izražen je kao zbroj doprinosa čvorova. Dana je također rekurzivna formula za račun Hosoya-Wienerovog polinoma uteženih stabala.