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HOSOYA POLYNOMIAL AND THE DISTANCE OF THE TOTAL GRAPH OF A TREE

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Let G be a connected graph possessing $d(G,k)$ vertex pairs at distance k. Its Hosoya polynomial is $H(G,\lambda) = \sum_{k\geq 1} d(G,k)\,\lambda^k$. The distance $d(G)$ of the graph G is the sum of distances of all pairs of its vertices, i. e., $d(G) = H'(G,1)$. Let $T(G)$ be the total graph of G. If G is a tree, then the Hosoya polynomial of $T(G)$ (as well as of several other graphs derived from G) is expressed in terms of $H(G,\lambda)$. As a consequence, a linear relation exists between $d(T(G))$ and $d(G)$.

1. INTRODUCTION

The graph polynomial which we study in this paper was invented in 1988 by HOSOYA [**1**] (and was originally named the WIENER *polynomial*). We nevertheless call it the HOSOYA *polynomial*. It is defined as follows.

Let G be a connected graph on n vertices. The vertex and edge sets of G are $V(G) = \{x_1, x_2, \ldots, x_n\}$ and $E(G) = \{y_1, y_2, \ldots, y_m\}$, respectively. The length (= number of edges) of a shortest path between the vertices $x_i, x_j \in V(G)$ is their *distance* and is denoted by $d(x_i, x_j|G)$. The number of (unordered) pairs of vertices of G, whose distance is k, is denoted by $d(G,k)$.

Let D be the diameter of the graph G. Clearly, $d(G,k) = 0$ whenever $k > D$. Furthermore, $d(G,k) > 0$ for all $k = 1, \ldots, D$ and $\sum_{k=1}^{D} d(G,k) = n(n-1)/2$.

Definition 1. *The* HOSOYA *polynomial of G is*

$$H(G) = H(G,\lambda) = \sum_{k=1}^{D} d(G,k)\,\lambda^k \tag{1}$$

or, what is the same,

$$H(G) = H(G,\lambda) = \sum_{1\leq i<j\leq n} \lambda^{d(x_i,\ x_j|G)}. \tag{2}$$

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Definition 2. *The distance $d(G)$ of the graph G (sometimes called the* Wiener *number) is equal to the sum of distances of all pairs of vertices of G,*

$$d(G) = \sum_{1 \le i < j \le n} d(x_i, x_j | G).$$

Combining Definitions 1 and 2 one immediately concludes that [**1**]

$$d(G) = \sum_{k=1}^{D} k\, d(G, k)$$

i. e.,

$$d(G) = H'(G, 1) \tag{3}$$

where $H'(G, \lambda)$ stands for the first derivative of $H(G, \lambda)$ with respect to λ.

We now define the following five types of graphs, derived from G.

1. The *line graph* $L(G)$ of G has as vertices the edges $y_1, y_2, \dots, y_m$ of G, $V(L(G)) = E(G)$. Two vertices of $L(G)$ are adjacent if, and only if, the respective edges of G are incident.

2. The *subdivision graph* $S(G)$ of G is obtained by inserting a new vertex on each edge of G. The subdivision graph can be viewed as consisting of the vertices of both G and $L(G)$, $V(S(G)) = V(G) \cup V(L(G))$. In view of this we denote the vertices of $S(G)$ by $x_1, x_2, \dots, x_n, y_1, y_2, \dots, y_m$ and say that the vertices $x_1, x_2, \dots, x_n$ originate from G whereas the vertices $y_1, y_2, \dots, y_m$ originate from $L(G)$.

The vertices of the below described semi-total graphs and of the total graph are labeled in the same manner as the vertices of the subdivision graph.

3. The *first semi-total graph* $ST_1(G)$ of G is obtained by adding new edges to $S(G)$, connecting all pairs of vertices originating from G and being adjacent in G. Thus $V(ST_1(G)) = V(S(G))$ and $E(ST_1(G)) = E(S(G)) \cup E(G)$.

4. The *second semi-total graph* $ST_2(G)$ of G is obtained by adding new edges to $S(G)$, connecting all pairs of vertices originating from $L(G)$ and being adjacent in $L(G)$. Thus $V(ST_2(G)) = V(S(G))$ and $E(ST_2(G)) = E(S(G)) \cup E(L(G))$.

5. The *total graph* $T(G)$ of G is obtained by adding new edges to $S(G)$, connecting all pairs of vertices originating from G and being adjacent in G and all pairs of vertices originating from $L(G)$ and being adjacent in $L(G)$. Thus $V(T(G)) = V(S(G))$ and $E(T(G)) = E(S(G)) \cup E(G) \cup E(L(G))$.

An illustrative example is provided in Fig. 1.

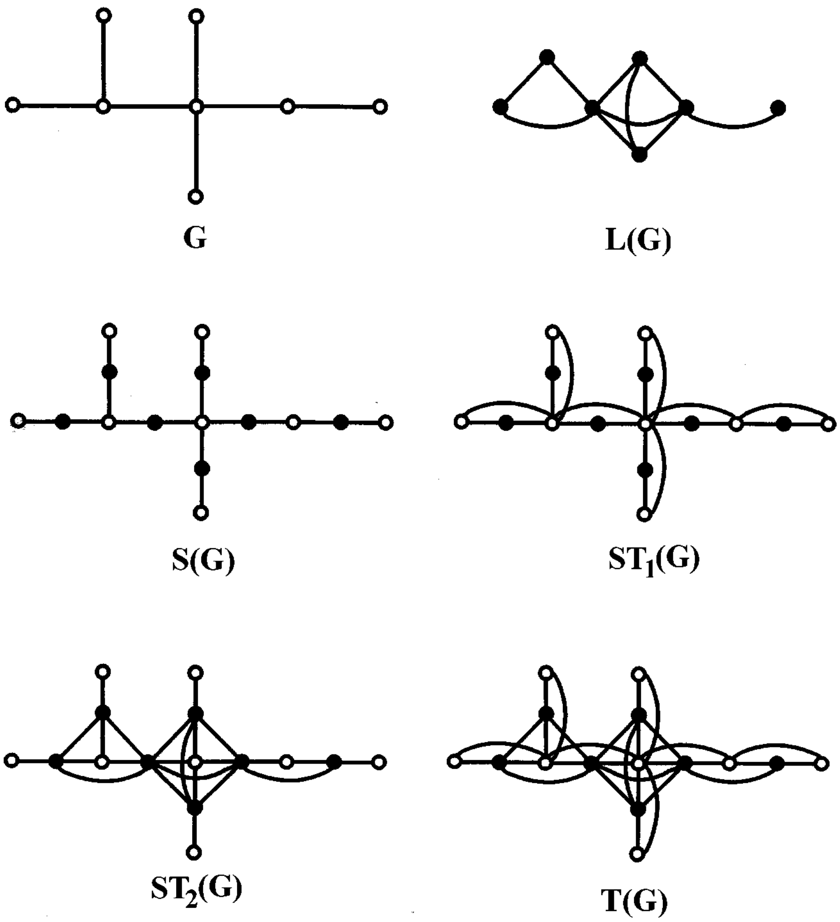

Fig. 1.

2. STATEMENT OF THE RESULTS

Let, as before, G be a connected graph on n vertices and let $L(G)$, $S(G)$, $ST_1(G)$, $ST_2(G)$ and $T(G)$ be respectively the line graph, the subdivision graph, the first and second semi-total graph and the total graph of G.

Theorem 1. *If G is an n-vertex tree, then:*

$$H(L(G),\lambda) = \frac{1}{\lambda}\, H(G,\lambda) - (n-1), \tag{4}$$

$$H(S(G),\lambda) = \left(1 + \frac{1}{\lambda}\right)^2 H(G,\lambda^2) - (n-1), \tag{5}$$

$$H(ST_1(G),\lambda) = 4\,H(G,\lambda) - (n-1)\lambda, \tag{6}$$

$$H(ST_2(G),\lambda) = \lambda\left(1+\frac{1}{\lambda}\right)^2 H(G,\lambda) - (n-1), \tag{7}$$

$$H(T(G),\lambda) = \left(3+\frac{1}{\lambda}\right) H(G,\lambda) - (n-1). \tag{8}$$

Theorem 2. *If G is an n-vertex tree, then the distances of $L(G)$, $S(G)$, $ST_1(G)$, $ST_2(G)$ and $T(G)$ are all simple linear functions of the distance of G:*

$$d(L(G)) = d(G) - \frac{1}{2}\,n(n-1), \tag{9}$$

$$d(S(G)) = 8\,d(G) - 2n(n-1), \tag{10}$$

$$d(ST_1(G)) = 4\,d(G) - (n-1), \tag{11}$$

$$d(ST_2(G)) = 4\,d(G), \tag{12}$$

$$d(T(G)) = 4\,d(G) - \frac{1}{2}\,n(n-1). \tag{13}$$

It should be noted that none of the relations (4)–(13) is, in the general case, obeyed for cycle–containing graphs. In particular, all these relations are violated if G is chosen to be the triangle.

A formula equivalent to (9) was earlier reported by BUCKLEY [**2**].

3. PROOF OF THEOREMS 1 AND 2

Throughout this section it is assumed that G is an n-vertex tree. Hence, $m = n-1$.

In order to deduce Eq. (4) recall [**2**], [**3**] that in the case of trees there exists a one–to–one correspondence between the shortest paths of length k of $L(G)$ and the paths of length $k+1$ of G, $k = 1,2,\ldots$. Therefore for $k \geq 1$, $d(L(G),k) = d(G,k+1)$. Formula (4) follows now directly from the definition (1) of the HOSOYA polynomial and the fact that $d(G,1) = |E(G)| = n-1$.

In order to deduce Eqs. (5)–(8) it is convenient to refer to the vertices $x_1, x_2, \ldots, x_n$ of $S(G), ST_1(G), ST_2(G)$ and $T(G)$ as white and to the vertices $y_1, y_2, \ldots, y_m$ as black, cf. Fig. 1.

In view of Eq. (2), the HOSOYA polynomial of $S(G)$ is decomposed into three terms, namely into contributions of pairs of white vertices (P_{ww}), pairs of black vertices (P_{bb}) and pairs of differently colored vertices (P_{wb}):

$$H(S(G)) = P_{ww} + P_{bb} + P_{wb} \tag{14}$$

where

$$P_{ww} = \sum_{1\leq i<j\leq n} \lambda^{d(x_i,\ x_j|S(G))},\quad P_{bb} = \sum_{1\leq r<s\leq m} \lambda^{d(y_r,\ y_s|S(G))},$$

$$P_{wb} = \sum_{i=1}^{n} \sum_{r=1}^{m} \lambda^{d(x_i,\ y_r|S(G))}.$$

From the construction of the subdivision graph it is evident that

$$d(x_i, x_j|S(G)) = 2\,d(x_i, x_j|G),\ d(y_r, y_s|S(G)) = 2\,d(y_r, y_s|L(G))$$

which implies

(15) $$P_{ww} = H(G, \lambda^2) \quad \text{and} \quad P_{bb} = H(L(G), \lambda^2)\ .$$

Consider now a pair of differently colored vertices of $S(G)$, say x_i and y_r. Because $S(G)$ is a tree, there is a unique path π_{ir}, connecting x_i and y_r. Let $y_{r'}$ be the vertex of $S(G)$, belonging to π_{ir} and being adjacent to x_i. Let $x_{i'}$ be the vertex of $S(G)$, not belonging to π_{ir} and being adjacent to y_r. Both $x_{i'}$ and $y_{r'}$ are uniquely determined by x_i and y_r.

Now, the distance between $x_i, y_r \in V(S(G))$ is by one smaller than the distance between $x_i, x_{i'} \in V(S(G))$, which on the other hand is twice the distance between $x_i, x_{i'} \in V(G)$. Because the same is true also for the vertex pair $x_{i'}, y_{r'} \in V(S(G))$, we arrive at the conclusion that

(16) $$P_{wb} = 2 \sum_{1 \le i < i' \le n} \lambda^{d(x_i,\ x_{i'}|S(G))-1} = 2 \sum_{1 \le i < j \le n} \lambda^{2\,d(x_i,\ x_{i'}|G)-1} = \frac{2}{\lambda} H(G, \lambda^2)\ .$$

Substituting (15) and (16) back into (14) we obtain

(17) $$H(S(G), \lambda) = H(G, \lambda^2) + H(L(G), \lambda^2) + \frac{2}{\lambda} H(G, \lambda^2)\ .$$

Combining (17) with (4) yields (5).

The derivation of formulas (6)–(8) is analogous. For instance, in the case of the total graph, for any pair of white vertices

(18) $$d(x_i, x_j|T(G)) = d(x_i, x_j|G)$$

whereas for any pair of black vertices

(19) $$d(y_r, y_s|T(G)) = d(y_r, y_s|L(G))\ .$$

Using the above specified notation, for the pairs $x_i, y_r \in V(T(G))$ and $x_{i'}, y_{r'} \in V(T(G))$ of differently colored vertices,

(20) $$d(x_i, y_r|T(G)) = d(x_{i'}, y_{r'}|T(G)) = d(x_i, x_{i'}|G)\ .$$

From (18)–(20) follows

$$H(T(G), \lambda) = H(G, \lambda) + H(L(G), \lambda) + 2\,H(G, \lambda)$$

and Eq. (8) is obtained using (4).

This completes the proof of Theorem 1.

The results collected in Theorem 2 are direct corollaries of formulas (4)–(8), obtained by differentiating the HOSOYA polynomials with respect to λ, by applying Eq. (3) and by bearing in mind that $H(G,1) = n(n-1)/2$.

4. DISCUSSION

Theorems 1 and 2 show that for a large number of graphs, constructed from a tree and being in a one–to–one correspondence with this tree, the HOSOYA polynomials and the distances are mutually related. In particular, the distances are related in a linear manner.

Results of the same kind (for other types of graphs derived from trees) were recently reported [**4**], and still more such results were obtained by the author. Of them we state without proof the following.

Let $S_p(G)$ be the p-th subdivision graph of the graph G, obtained by inserting p vertices on each edge of G. If G is an n-vertex tree, then

$$d(S_p(G)) = (p+1)^3\, d(G) - \frac{1}{2}\, p(p+1)^2\, n(n-1) + \frac{1}{6}\, p(p-1)(p+1)(n-1)\ .$$

For $p = 1$ the above formula reduces to Eq. (10).

It may well happen that all these relations are just special cases of some more general connection between distance–based invariants of graphs derived from trees. The possible discovery of this connection remains a task for the future.

Another task for the future is to find an explanation why nice results, as those stated in Theorems 1 and 2, hold for distance–based invariants of graphs originating from trees (which, nevertheless, may possess cycles), but do not hold for graphs constructed in an analogous manner from cycle–containing graphs.

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