Bulletin T.CXXXI de l'Académie serbe des sciences et des arts − 2005
Classe des Sciences mathématiques et naturelles
Sciences mathématiques, № 30

SOME RELATIONS BETWEEN DISTANCE–BASED POLYNOMIALS OF TREES

I. GUTMAN

(Presented at the 6th Meeting, held on September 24, 2004)

A b s t r a c t. *The Hosoya polynomial $H(G,\lambda)$ of a graph G has the property that its first derivative at $\lambda = 1$ is equal to the Wiener index. Sometime ago two distance-based graph invariants were studied – the Schultz index S and its modification S^*. We construct distance–based graph polynomials $H_1(G,\lambda)$ and $H_2(G,\lambda)$, such that their first derivatives at $\lambda = 1$ are, respectively, equal to S and S^*. In case of trees, $H_1(G,\lambda)$ and $H_2(G,\lambda)$ are related with $H(G,\lambda)$.*

AMS Mathematics Subject Classification (2000): 05C12, 05C05
Key Words: Graph polynomial, distance (in graph), tree, Wiener index, Schultz index

1. *Introduction*

In this work we study some distance–based graph invariants and polynomials, and find relations between them. Let G be a connected graph, $V(G)$ its vertex set, n the number of its vertices, and m the number of its edges.

Let x and y be vertices of the graph G. The distance $d(x,y)$ between them (equal to the length of the shortest path connecting them) is denoted by $d(x,y)$. If $x = y$, then $d(x,y) = 0$. The number of pairs of vertices of G that are at distance k is denoted by $d(G,k)$. In particular, $d(G,0) = n$, $d(G,1) = m$, and $\sum_{k \geq 0} d(G,k) = \binom{n}{2} + n = n(n+1)/2$.

The degree δ_x of the vertex x is the number of first neighbors of this vertex.

A much studied distance–based graph invariant is the *Wiener index*, defined as

$$W = W(G) = \sum_{\{x,y\} \subseteq V(G)} d(x,y) \tag{1}$$

which also can be written as

$$W = W(G) = \sum_{k \geq 0} k\, d(G,k) \ . \tag{2}$$

For details on the mathematical properties of the Wiener index see the reviews [1, 2].

Hosoya [3] introduced a distance–based graph polynomial

$$H(G,\lambda) = \sum_{k \geq 0} d(G,k)\, \lambda^k \tag{3}$$

nowadays called the "*Hosoya polynomial*". A less usual, yet equivalent, form in which this polynomial can be written is

$$H(G,\lambda) = \sum_{\{x,y\} \subseteq V(G)} \lambda^{d(x,y)} \ . \tag{4}$$

As easily seen from Eqs. (2) and (3) or from (1) and (4), the first derivative of the Hosoya polynomial at $\lambda = 1$ is equal to the Wiener index.

In connection with certain investigations in mathematical chemistry, Schultz [4] considered a graph invariant that he called "molecular topological index" and whose essential part is the *Schultz index* S ,

$$S = S(G) = \sum_{\{x,y\} \subseteq V(G)} (\delta_x + \delta_y)\, d(x,y) \ . \tag{5}$$

The Schultz index attracted some attention after it was discovered that in the case of trees it is closely related to the Wiener index [5]:

Theorem 1. *If G is a tree on n vertices, then its Schultz and Wiener indices are related as*

$$S(G) = 4\, W(G) - n(n-1) \ . \tag{6}$$

Motivated by Eqs. (5) and (6), the present author [6] examined an invariant S^*,

$$S^* = S^*(G) = \sum_{\{x,y\} \subseteq V(G)} \delta_x \, \delta_y \, d(x,y) \tag{7}$$

which here we refer to as the *modified Schultz index*. A result analogous to Theorem 1 applies [6]:

Theorem 2. *If G is a tree on n vertices, then its modified Schultz and Wiener indices are related as*

$$S^*(G) = 4\, W(G) - (n-1)(2n-1) \ . \tag{8}$$

2. *Graph Polynomials Related to the Schultz and Modified Schultz Indices*

Bearing in mind Eqs. (4), (5), and (7), it is easy to construct graph polynomials having the property that their first derivatives at $\lambda = 1$ are equal to the Schultz and modified Schultz indices. These polynomials are

$$H_1(G,\lambda) \quad = \sum_{\{x,y\} \subseteq V(G)} (\delta_x + \delta_y)\, \lambda^{d(x,y)} \tag{9}$$

$$H_2(G,\lambda) \quad = \sum_{\{x,y\} \subseteq V(G)} \delta_x \, \delta_y \, \lambda^{d(x,y)} \tag{10}$$

In view of Eqs. (6) and (8) one may ask if there exist relations between the polynomials H_1 and H_2 and the Hosoya polynomial, in particular in the case of trees. The answer to this question is affirmative, and we have

Theorem 3. *If G is a tree on n vertices, then the polynomials $H_1(G,\lambda)$ and $H(G,\lambda)$ are related as*

$$H_1(G,\lambda) = 2\left(1+\frac{1}{\lambda}\right) H(G,\lambda) - 2\left(1+\frac{n}{\lambda}\right) \ . \tag{11}$$

Theorem 4. *If G is a tree on n vertices, then the polynomials $H_2(G,\lambda)$ and $H(G,\lambda)$ are related as*

$$\begin{aligned} H_2(G,\lambda) \quad &= \quad \left(1+\frac{1}{\lambda}\right)^2 H(G,\lambda) - \left(1+\frac{1}{\lambda}\right)\left(2+\frac{1}{\lambda}\right) n \\ &+ \quad \left(1+\frac{1}{\lambda}\right) + \frac{1}{2} \sum_{x \in V(G)} (\delta_x)^2 \ . \end{aligned} \tag{12}$$

3. *Proof of Theorem 3*

Lemma 5. *If G is a tree, then*

$$\sum_{x \neq y} (\delta_x + \delta_y - 2)\, \lambda^{d(x,y)+1} = 2 \sum_{k \geq 2} d(G,k)\, \lambda^k, \tag{13}$$

where $\sum_{x \neq y}$ indicates summation over all pairs of different vertices x, y of G.

P r o o f. The sum

$$\sum_{x \neq y} (\delta_y - 1)\, \lambda^{d(x,y)+1}$$

can be viewed as going over all pairs of vertices x, z of the tree G, where z is adjacent to y and is at greater distance from x than y. Because G is a tree, there exist exactly $\delta_y - 1$ such vertices, and their distances to x are equal to $d(x,y) + 1$. In other words, the above sum is equal to the sum of the terms $\lambda^{d(x,z)}$ over all pairs of vertices of the tree G whose distance is 2 or greater, i. e.,

$$\sum_{x \neq y} (\delta_y - 1)\, \lambda^{d(x,y)+1} = \sum_{k \geq 2} d(G,k)\, \lambda^k \ . \tag{14}$$

By the very same argument,

$$\sum_{x \neq y} (\delta_x - 1)\, \lambda^{d(x,y)+1} = \sum_{k \geq 2} d(G,k)\, \lambda^k \ . \tag{15}$$

By adding (14) and (15) we obtain (13). $\square$

P r o o f of Theorem 3. Bearing in mind Lemma 5, we rewrite the right–hand side of (9) as

$$\begin{aligned} H_1(G,\lambda) &= \sum_{x \neq y} (\delta_x + \delta_y - 2)\, \lambda^{d(x,y)} + \sum_{x = y} (\delta_x + \delta_y - 2)\, \lambda^{d(x,y)} \\ &+ 2 \sum_{\{x,y\} \subseteq V(G)} \lambda^{d(x,y)} \ . \end{aligned} \tag{16}$$

Now, by Lemma 5,

$$\sum_{x \neq y} (\delta_x + \delta_y - 2)\, \lambda^{d(x,y)} = \frac{1}{\lambda} \sum_{k \geq 2} d(G,k)\, \lambda^k \ .$$

If $x = y$ then $d(x,y) = 0$ and the second term on the right–hand side of (16) is equal to

$$\sum_{x \in V(G)} (2\,\delta_x - 2) = 4m - 2n = 4(n-1) - 2n = 2n - 4\ .$$

By (4), the third term on the right–hand side of (16) is just twice the Hosoya polynomial.

We thus get

$$H_1(G,\lambda) = \frac{1}{\lambda} \sum_{k \geq 2} d(G,k)\,\lambda^k + (2n-4) + 2\,H(G,\lambda)\ .$$

Taking into account that

$$\sum_{k \geq 2} d(G,k)\,\lambda^k = \sum_{k \geq 0} d(G,k)\,\lambda^k - d(G,0) - d(G,1)\,\lambda = H(G,\lambda) - n - (n-1)\,\lambda$$

we directly arrive at formula (11). □

Formula (6) can now be obtained as a simple corollary of Theorem 3. Indeed, one just has to compute the first derivative of (11), set $\lambda = 1$, and use the relations $H(G,1) = n(n+1)$ and $H'(G,1) = W$.

4. *Proof of Theorem 4*

Lemma 6. *If G is a tree, then*

$$\sum_{x \neq y} (\delta_x - 1)(\delta_y - 1)\,\lambda^{d(x,y)+2} = \sum_{k \geq 3} d(G,k)\,\lambda^k\ . \tag{17}$$

P r o o f. The sum

$$\sum_{x \neq y} (\delta_x - 1)(\delta_y - 1)\,\lambda^{d(x,y)+2}$$

can be viewed as embracing all pairs of vertices z, z' of the tree G, where z is adjacent to x and is at greater distance from y than x, and z' is adjacent to y and is at greater distance from x than y. Because G is a tree, there exist exactly $\delta_x - 1$ vertices z and $\delta_y - 1$ vertices z', and thus a total of $(\delta_x - 1)(\delta_y - 1)$ vertex pairs z, z'. The distance of each such vertex pair is $d(x,y) + 2$. This implies that the above sum is equal to the sum of the terms $\lambda^{d(z,z')}$ over all pairs of vertices of the tree G whose distance is 3 or greater, i. e., implies Eq. (17)

P r o o f of Theorem 4. In view of Lemma 6, we rewrite the right-hand side of (10) as

$$\begin{aligned} H_2(G,\lambda) &= \sum_{x\neq y}(\delta_x-1)(\delta_y-1)\,\lambda^{d(x,y)} + \sum_{x=y}(\delta_x-1)(\delta_y-1)\,\lambda^{d(x,y)} \\ &+ \sum_{\{x,y\}\subseteq V(G)}(\delta_x+\delta_y)\,\lambda^{d(x,y)} - \sum_{\{x,y\}\subseteq V(G)}\lambda^{d(x,y)}\ . \end{aligned} \tag{18}$$

Then by Lemma 6,

$$\sum_{x\neq y}(\delta_x-1)(\delta_y-1)\,\lambda^{d(x,y)} = \frac{1}{\lambda^2}\sum_{k\geq 3} d(G,k)\,\lambda^k,$$

whereas the third and fourth terms on the right–hand side of (18) are just the polynomials $H_1(G,\lambda)$ and $H(G,\lambda)$, respectively. The second term in (18) is simply

$$\sum_{x\in V(G)}(\delta_x-1)^2 = \sum_{x\in V(G)}(\delta_x)^2 - 4m + n = \sum_{x\in V(G)}(\delta_x)^2 - 3n + 4\ .$$

Therefore,

$$H_2(G,\lambda) = \frac{1}{\lambda^2}\sum_{k\geq 3} d(G,k)\,\lambda^k + \sum_{x\in V(G)}(\delta_x)^2 - 3n + 4 + H_1(G,\lambda) - H(G,\lambda)\ .$$

By taking into account that

$$\sum_{k\geq 3} d(G,k)\,\lambda^k = H(G,\lambda) - n - (n-1)\,\lambda - d(G,2)\,\lambda^2,$$

recalling that in the case of trees [7]

$$d(G,2) = \frac{1}{2}\sum_{x\in V(G)}(\delta_x)^2 - (n-1),$$

and using the expression (11) for $H_1(G,\lambda)$, we arrive at Eq. (12), that is at Theorem 4. $\square$

Formula (8) becomes now a corollary of Theorem 4. It is obtained by setting $\lambda = 1$ into the first derivative of (12), using the relations (2) and (7), as well as $H(G,1) = n(n+1)$ and $H'(G,1) = W$.

REFERENCES

[1] A. A. D o b r y n i n, R. E n t r i n g e r, I. G u t m a n, *Wiener index of trees: theory and applications*, Acta Appl. Math. **66** (2001), 211–249.

[2] A. A. D o b r y n i n, I. G u t m a n, S. K l a v ž a r, P. Ž i g e r t, *Wiener index of hexagonal systems*, Acta Appl. Math. **72** (2002), 247–294.

[3] H. H o s o y a, *On some counting polynomials in chemistry*, Discr. Appl. Math. **19** (1988), 239–257.

[4] H. P. S c h u l t z, *Topological organic chemistry. 1. Graph theory and topological indices of alkanes*, J. Chem. Inf. Comput. Sci. **29**, (1989) 227–228.

[5] D. J. K l e i n, Z. M i h a l i ć, D. P l a v š i ć, N. T r i n a j s t i ć, *Molecular topological index: A relation with the Wiener index*, J. Chem. Inf. Comput. Sci. **32**, (1992) 304–305.

[6] I. G u t m a n, *Selected properties of the Schultz molecular topological index*, J. Chem. Inf. Comput. Sci. **34**, (1994) 1087–1089.

[7] I. G u t m a n, K. C. D a s, *The first Zagreb index 30 years after*, MATCH Commun. Math. Comput. Chem. **50**, (2004) 83–92.

Faculty of Science
University of Kragujevac
P. O. Box 60
34000 Kragujevac
Serbia and Montenegro