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INEQUALITIES BETWEEN DISTANCE–BASED GRAPH POLYNOMIALS

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A b s t r a c t. In a recent paper [I. Gutman, Bull. Acad. Serbe Sci. Arts (Cl. Math. Natur.) **131** (2005) 1–7], *the Hosoya polynomial* $H = H(G, \lambda)$ *of a graph* G *, and two related distance–based polynomials* $H_1 = H_1(G, \lambda)$ *and* $H_2 = H_2(G, \lambda)$ *were examined. We now show that*

$$\max\{\delta\, H_1 - \delta^2\, H\,,\ \Delta\, H_1 - \Delta^2\, H\} \leq H_2 \leq \Delta\, H_1 - \delta\,\Delta\, H$$

holds for all graphs G *and for all* $\lambda \geq 0$ *, where* δ *and* Δ *are the smallest and greatest vertex degree in* G *. The answer to the question which of the terms* $\delta\, H_1 - \delta^2\, H$ *and* $\Delta\, H_1 - \Delta^2\, H$ *is greater, depends on the graph* G *and on the value of the variable* λ *. We find a number of particular solutions of this problem.*

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1. *Introduction*

In a recent paper [1] some distance–based graph polynomials were studied and relations between them established. We now obtain inequalities between these polynomials.

We use the same notation and terminology as in [1]: By G is denoted a connected graph, $V(G)$ its vertex set, $E(G)$ its edge set, n the number of its vertices, and m the number of its edges. By δ_x is denoted the degree of the vertex $x \in V(G)$. The smallest and greatest vertex degree in the graph G are δ and Δ, respectively.

The distance between the vertices x and y of the graph G is denoted by $d(x,y)$. Because the graph G is assumed to be connected, the distance $d(x,y)$ is a well-defined quantity for all pairs of vertices x and y. In particular, if $x = y$, then $d(x,y) = 0$. The greatest distance in G is its diameter and will be denoted by D. The number of pairs of vertices of G that are at distance k is denoted by $d(G,k)$.

The Hosoya polynomial (originally called "Wiener polynomial" [2]) of a graph G is defined as

$$H = H(G,\lambda) = \sum_{k \geq 0} d(G,k)\,\lambda^k \ . \tag{1}$$

This graph polynomial was much studied in the past [3–10].

Another way in which the right–hand side of Eq. (1) can be written is

$$H(G,\lambda) = \sum_{\{x,y\} \subseteq V(G)} \lambda^{d(x,y)} \ . \tag{2}$$

The expression (2) made it possible [1] to conceive two other, closely related graph polynomials, viz.,

$$H_1 = H_1(G,\lambda) = \sum_{\{x,y\} \subseteq V(G)} (\delta_x + \delta_y)\,\lambda^{d(x,y)} \tag{3}$$

and

$$H_2 = H_2(G,\lambda) = \sum_{\{x,y\} \subseteq V(G)} \delta_x\,\delta_y\,\lambda^{d(x,y)} \ . \tag{4}$$

Let $P = P(\lambda)$ be a polynomial of the form

$$P(\lambda) = \sum_{k=0}^{n} a_k\,\lambda^k$$

Then we write $a_k = \texttt{coeff}_k(P)$. With this notation, in view of Eqs. (2) and (3), it is elementary to verify the following:

$$\texttt{coeff}_0(H) = n \qquad ; \qquad \texttt{coeff}_1(H) = m \tag{5}$$

$$\texttt{coeff}_0(H_1) = 4m \qquad ; \qquad \texttt{coeff}_1(H_1) = \sum_{x \in V(G)} (\delta_x)^2 \ . \tag{6}$$

The second relation in (6) is a consequence of

$$\sum_{xy \in E(G)} (\delta_x + \delta_y) = \sum_{x \in V(G)} (\delta_x)^2 \ .$$

A graph is said to be regular of degree r if all its vertices have degrees equal to r. In this case the above defined graph polynomials are simply related as

$$H_1 = 2r\, H \qquad \text{and} \qquad H_2 = r^2\, H \ .$$

In view of this, in what follows we shall assume that the graphs considered are non-regular, which is tantamount to the requirement $\delta < \Delta$.

2. *Elementary Inequalities between the Polynomials H, H_1, and H_2*

For any vertex $x \in V(G)$, $\delta \le \delta_x \le \Delta$. Therefore, for any pair of (not necessarily distinct) vertices $x, y \in V(G)$,

$$(\delta_x - \delta)(\delta_y - \delta) \ \ge \ 0 \tag{7}$$

$$(\delta_x - \Delta)(\delta_y - \Delta) \ \ge \ 0 \tag{8}$$

$$(\delta_x - \delta)(\delta_y - \Delta) \ \le \ 0 \ . \tag{9}$$

From (7) and (8) there follows

$$\delta_x\, \delta_y - \delta\, (\delta_x + \delta_y) + \delta^2 \ \ge \ 0$$

$$\delta_x\, \delta_y - \Delta\, (\delta_x + \delta_y) + \Delta^2 \ \ge \ 0,$$

which in view of Eqs. (2)–(4) and assuming that $\lambda \ge 0$ immediately yields

$$H_2 - \delta\, H_1 + \delta^2\, H \ \ge \ 0 \tag{10}$$

$$H_2 - \Delta\, H_1 + \Delta^2\, H \ \ge \ 0 \ . \tag{11}$$

From (9) one obtains

$$\delta_x\, \delta_y - (\Delta\, \delta_x + \delta\, \delta_y) + \delta\, \Delta \le 0$$

from which there follows a weaker inequality

$$\delta_x\, \delta_y - \Delta\, (\delta_x + \delta_y) + \delta\, \Delta \le 0$$

which, in turn, implies

$$H_2 - \Delta\, H_1 + \delta\, \Delta\, H \le 0 \ . \tag{12}$$

Bearing in mind the inequalities (10)–(12) we have

Theorem 1. *Let δ and Δ be, respectively, the smallest and the greatest vertex degree in the graph G. Then for any connected graph G and all $\lambda \geq 0$,*

$$\max\{\delta\, H_1(G,\lambda) - \delta^2\, H(G,\lambda)\,,\, \Delta\, H_1(G,\lambda) - \Delta^2\, H(G,\lambda)\} \;\leq\; H_2(G,\lambda) \\ \leq\; \Delta\, H_1(G,\lambda) - \delta\,\Delta\, H(G,\lambda)\ .$$

Finding which of the two terms in the lower bound in Theorem 1 is greater, appears to be a difficult task. Anyway, it is either

$$\max\{\delta\, H_1 - \delta^2\, H\,,\, \Delta\, H_1 - \Delta^2\, H\} = \delta\, H_1 - \delta^2\, H \tag{13}$$

or

$$\max\{\delta\, H_1 - \delta^2\, H\,,\, \Delta\, H_1 - \Delta^2\, H\} = \Delta\, H_1 - \Delta^2\, H\ . \tag{14}$$

Comparing the right–hand sides of (13) and (14), and taking into account that $\Delta - \delta > 0$, we arrive at the following auxiliary

Lemma 2. *If $(\delta + \Delta)\, H(G,\lambda) > H_1(G,\lambda)$, then Eq. (13) holds. If $(\delta + \Delta)\, H(G,\lambda) < H_1(G,\lambda)$, then Eq. (14) holds. If $(\delta + \Delta)\, H(G,\lambda) = H_1(G,\lambda)$, then both Eqs. (13) and (14) are applicable.*

If Eqs. (13) and (14) simultaneously hold, then

$$(\delta + \Delta)\, H(G,\lambda) - H_1(G,\lambda) = 0\ . \tag{15}$$

The real non-negative solutions of Eq. (15) (if any) will be referred to as the critical values of the graph G.

In what follows we examine the conditions for the validity of (13) and (14). The following example reveals that these conditions are far from being trivial.

Example 1. Let P_n be the n-vertex path and let $n \geq 3$. Then $\delta = 1$ and $\Delta = 2$. It can be shown that

$$H(P_n,\lambda) = \sum_{k=0}^{n-1} (n-k)\,\lambda^k \qquad \text{and} \qquad H_1(P_n,\lambda) = 4n-4+\sum_{k=1}^{n-1} (4n-2-4k)\,\lambda^k\ .$$

Thus, in the case $n = 3$,

$$\begin{aligned} (\delta + \Delta)\, H(P_n,\lambda) &= 9 + 6\,\lambda + 3\,\lambda^2 \\ H_1(P_n,\lambda) &= 8 + 6\,\lambda + 2\,\lambda^2 \end{aligned}$$

and thus Eq. (13) holds for all values of the variable λ, $\lambda \geq 0$. The path P_3 has no critical values.

In the case $n = 4$ we have

$$\begin{aligned}(\delta + \Delta)\, H(P_n, \lambda) &= 12 + 9\,\lambda + 6\,\lambda^2 + 3\,\lambda^3 \\ H_1(P_n, \lambda) &= 12 + 10\,\lambda + 6\,\lambda^2 + 2\,\lambda^3 \,.\end{aligned}$$

Consequently, Eq. (14) holds for near-zero (positive) values of the variable λ, whereas (13) holds if λ is sufficiently large. By a detailed examination we find that Eq. (14) holds for $0 < \lambda < 1$, and Eq. (13) holds for $\lambda > 1$. The path P_4 has two critical values, $\lambda_1(P_4) = 0$ and $\lambda_2(P_4) = 1$.

In the case $n = 5$ the situation is slightly different: (14) holds for $0 \leq \lambda < \lambda_1$, (13) holds for $\lambda > \lambda_1$, and there is only a single critical value $\lambda_1(P_5) = (1 + \sqrt{5})/2$.

The problem of establishing which of the Eqs. (13) and (14) is valid becomes much less perplexed if one restricts the consideration to near zero (positive) and to very large values of the variable λ.

Lemma 3. *If λ is sufficiently close to zero (but positive–valued), then*

$$(\delta + \Delta)\, \texttt{coeff}_0(H) > \texttt{coeff}_0(H_1) \tag{16}$$

implies the validity of Eq. (13), and

$$(\delta + \Delta)\, \texttt{coeff}_0(H) < \texttt{coeff}_0(H_1) \tag{17}$$

implies the validity of Eq. (14). If

$$(\delta + \Delta)\, \texttt{coeff}_0(H) = \texttt{coeff}_0(H_1) \tag{18}$$

then

$$(\delta + \Delta)\, \texttt{coeff}_1(H) > \texttt{coeff}_1(H_1) \tag{19}$$

implies the validity of Eq. (13), and

$$(\delta + \Delta)\, \texttt{coeff}_1(H) < \texttt{coeff}_1(H_1) \tag{20}$$

implies the validity of Eq. (14). If also

$$(\delta + \Delta)\, \texttt{coeff}_1(H) = \texttt{coeff}_1(H_1) \tag{21}$$

then one has to compare the second coefficients of $H(G, \lambda)$ and $H_1(G, \lambda)$, etc.

With regard to conditions (18)–(21) see Lemma 5.

Lemma 4. *Let D be the diameter of the graph G under consideration. If λ is sufficiently large, then*

$$(\delta + \Delta)\,\texttt{coeff}_D(H) > \texttt{coeff}_D(H_1) \tag{22}$$

implies the validity of Eq. (13), and

$$(\delta + \Delta)\,\texttt{coeff}_D(H) < \texttt{coeff}_D(H_1)$$

implies the validity of Eq. (14). If

$$(\delta + \Delta)\,\texttt{coeff}_D(H) = \texttt{coeff}_D(H_1)$$

then

$$(\delta + \Delta)\,\texttt{coeff}_{D-1}(H) > \texttt{coeff}_{D-1}(H_1)$$

implies the validity of Eq. (13), and

$$(\delta + \Delta)\,\texttt{coeff}_{D-1}(H) < \texttt{coeff}_{D-1}(H_1)$$

implies the validity of Eq. (14). If also

$$(\delta + \Delta)\,\texttt{coeff}_{D-1}(H) = \texttt{coeff}_{D-1}(H_1)$$

then one has to compare the third-last coefficients of $H(G,\lambda)$ and $H_1(G,\lambda)$, etc.

Lemma 5. *For any connected and non-regular graph, the validity of Eq. (18) implies the validity of (20), i.e., if (18) holds, then conditions (19) and (21) never occur.*

P r o o f. Bearing in mind (5) and (6) we immediately see that (18) is equivalent to

$$(\delta + \Delta)\, n = 4m. \tag{23}$$

Now, knowing that $\sum\limits_{x \in V(G)} \delta_x = 2m$, we have

$$\sum_{x \in V(G)} (\delta_x)^2 = \sum_{x \in V(G)} \left(\delta_x - \frac{2m}{n}\right)^2 + \frac{4m^2}{n}$$

which (for non-regular graphs) implies

$$\sum_{x \in V(G)} (\delta_x)^2 > \frac{4m^2}{n} .$$

Combining this inequality with (23), we get

$$\sum_{x \in V(G)} (\delta_x)^2 > (\delta + \Delta)\, m$$

which is equivalent with (20). $\square$

* * * * *

Relation (23) determines the condition under which a graph has a critical value equal to zero.

In the case of trees, $\delta = 1$, $m = n - 1$, and (23) becomes

$$(3 - \Delta)n = 4 .$$

This condition is obeyed only if $\Delta = 2$ and $n = 4$, i.e., among all trees only the 4-vertex path has a zero critical value.

In the case of unicyclic graphs (different from C_n), $\delta = 1$ and $m = n$. Then from (23) follows $\Delta = 3$. Thus, connected unicyclic graphs with maximum vertex degree 3 have a zero critical value. Those with maximum vertex degree greater than 3 have no such critical value.

In the case of bicyclic graphs, $m = n + 1$ and (23) yields

$$(\delta + \Delta - 4)n = 4 .$$

This equality has solution only if $n = 4$, $\delta = 2$, $\Delta = 3$, which characterizes a unique graph (obtained by inserting an edge into C_4). Thus $C_4 + e$ is the unique bicyclic graph with a zero critical value.

In the case of tricyclic graphs we arrive at the condition $(\delta + \Delta - 4)n = 8$ which is satisfied by numerous graphs, all having $n = 8$, $\delta = 1$, $\Delta = 4$ or $n = 8$, $\delta = 2$, $\Delta = 3$.

3. *Trees*

In the case of trees the minimum vertex degree is always $\delta = 1$. The only n-vertex tree with $\Delta = 2$ is the path P_n , and this graph has already been analyzed in Example 1. Therefore we consider here trees for which $\Delta \geq 3$. Thus $\delta + \Delta \geq 4$.

An n-vertex tree has $n-1$ edges. Then, as special cases of Eqs. (5) and (6) we get

$$\texttt{coeff}_0(H) = n \qquad ; \qquad \texttt{coeff}_0(H_1) = 4(n-1)$$

and therefore relation (16) in Lemma 3 is satisfied. This, together with Example 1, implies

Theorem 6a. *Let G be an n-vertex tree. If $G \cong P_n$, $n \geq 4$, then Eq. (14) holds for near-zero values of λ. For all other n-vertex trees, $n \geq 3$, including P_3, Eq. (13) holds for near-zero values of λ.*

If λ is sufficiently large, then the leading term of the polynomial $H(G, \lambda)$ becomes $d(G, D)\, \lambda^D$, where $d(G, D)$ is the number of pairs of vertices at greatest distance. If G is a tree, then all pairs of its vertices at greatest distance are of degree 1, and therefore for large λ the leading term of the polynomial $H_1(G, \lambda)$ is $2\, d(G, D)\, \lambda^D$. Because for any n-vertex tree, $n \geq 3$, $\delta + \Delta \geq 3$, it immediately follows that all trees (including the paths) satisfy the condition (22) in Lemma 4. We thus arrive at

Theorem 6b. *For all n-vertex trees, $n \geq 3$, Eq. (13) holds for sufficiently large values of λ.*

4. *Unicyclic Graphs*

In this section we consider connected unicyclic graphs on n vertices. The cycle C_n is a regular graph of degree 2 and (for reasons explained above) will be disregarded. All other such graphs possess vertices of degree 1, and thus $\delta = 1$ and $\Delta \geq 3$. For connected unicyclic graphs, $n = m$, and therefore from Eqs. (5) and (6) we conclude that

$$\texttt{coeff}_0(H) = n \qquad ; \qquad \texttt{coeff}_0(H_1) = 4n \ . \tag{24}$$

We separately consider two cases: (1) $\Delta = 3$ and (2) $\Delta > 3$.

Case 1: $\Delta = 3$
Because of $\delta + \Delta = 4$ and relations (24), the equality (18) in Lemma 3 holds. Then, by Lemma 5 there follows that relation (20) in Lemma 3 is satisfied.

Case 2: $\Delta > 4$

This time from Eqs. (24) we conclude

$$(\delta + \Delta)\,\mathtt{coeff}_0(H) > 4n = \mathtt{coeff}_0(H_1),$$

which means that relation (16) in Lemma 3 is obeyed. Summarizing the above consideration we have

Theorem 7a. *Let G be an n-vertex connected unicyclic graph, different from the cycle C_n. If the greatest vertex degree in G is $\Delta = 3$, then Eq. (14) holds for near-zero values of λ. If $\Delta \geq 4$, then Eq. (13) holds for near-zero values of λ.*

Let G be a connected unicyclic graph on n vertices, different from C_n, and let D be its diameter. Let x and y be two vertices of G whose distance is D. The following properties of these vertices are easily verified:

Claim 1. Either $\delta_x = 1$ or $\delta_y = 1$, or both.
Claim 2. If $\delta_x = 1$, then $\delta_y \leq 2$.

P r o o f. Any unicyclic graph G (different from C_n) consists of a cycle C to which some trees are attached.

Without loss of generality we assume that $d(x, y) = D$ and $\delta_x \leq \delta_y$. We prove the Claims 1 and 2 by showing that the assumptions (a) $\delta_x > 1$ and (b) $\delta_x = 1$, $\delta_y > 2$ lead to contradictions.

Case (a): $\delta_x > 1$.

If x belongs to a tree, attached to the cycle C, then (because its distance to y is maximal), it must be $\delta_x = 1$. Therefore, x must belong to the cycle C.

If x belongs to the cycle C and has degree greater than 2, then a tree is attached to C at vertex x. The vertex y cannot belong to this tree, because then the distance between y and any vertex of C, different than x, would be greater than D, a contradiction. If so, then the distance between y and any vertex of the tree attached to x is greater than D, a contradiction. Therefore it cannot be $\delta_x > 2$.

Therefore, if x belongs to the cycle C, its degree would have to be equal to 2. Because, $\delta_y \geq \delta_x$, also the vertex y must belong to C.

If $\delta_y > 2$, then a tree is attached to y and the distance between x and any vertex of this tree is greater than D, a contradiction. If, however, $\delta_y = 2$, then on the cycle C there exists another pair of vertices x', y' at the same distance as x, y, such that a tree is attached to y'. The distance between

x' and any vertex of the tree attached to y' would be greater than D, a contradiction.

Therefore, it cannot be $\delta_x > 1$.

Case (b): $\delta_x = 1$, $\delta_y > 2$.

If $\delta_x = 1$, then x belongs to a tree attached to C. If $\delta_y > 2$, then y must belong to C, and a tree is attached to C at y. Then the distance between x and at least one neighbor of y would be greater that D, a contradiction.

Therefore, if $\delta_x = 1$, then it cannot be $\delta_y > 2$. □

The above stated properties of maximum–distance vertex pairs imply $\delta_x + \delta_y \leq 3$, from which follows that

$$\texttt{coeff}_D(H_1) \leq 3\, d(G, D) \ .$$

On the other hand, because of $\delta + \Delta \geq 4$,

$$(\delta + \Delta)\, \texttt{coeff}_D(H) \geq 4\, d(G, D)$$

which means that condition (22) in Lemma 4 is obeyed. This results in:

Theorem 7b. *For all connected unicyclic n-vertex graphs, $n \geq 4$, different from the cycle C_n, Eq. (13) holds for sufficiently large values of λ.*

5. *Hexagonal Systems*

Hexagonal systems form a class of graphs that is of certain importance in chemical applications; in chemical literature these graphs are often referred to as "benzenoid systems". The basic properties of hexagonal systems are systematized in the book [11]; for their distance–based properties see the review [12] and elsewhere [10].

The basic structural features of hexagonal systems are best described by the following parameters: number of hexagons h and number of internal vertices n_i. Recall that n_i is equal to the number of vertices that simultaneously belong to three hexagons. Then the number of vertices and edges is equal to [11] $n = 4h + 2 - n_i$ and $m = 5h + 1 - n_i$.

Hexagonal systems possess only vertices of degree 2 and 3. Their number is [11] $n_2 = 2h + 4 - n_i$ and $n_3 = 2h - 2$, respectively. Taking these relations into account, and noting that

$$\sum_{x \in V(G)} (\delta_x)^2 = 4\, n_2 + 9\, n_3,$$

we arrive at the following special cases of Eqs. (5) and (6):

$$\texttt{coeff}_0(H) = 4h + 2 - n_i \qquad ; \qquad \texttt{coeff}_1(H) = 5h + 1 - n_i$$
$$\texttt{coeff}_0(H_1) = 20\,h + 4 - 4\,n_i \qquad ; \qquad \texttt{coeff}_1(H_1) = 26\,h + 28 - 9\,n_i\ .$$

The hexagonal systems with $h = 1$ coincides with the 6-vertex cycle, which is a regular graph. Therefore, in what follows we assume that $h \geq 2$. If so, then $\delta = 2$ and $\Delta = 3$. Then, by direct calculation, we conclude that Eqs. (16) and (17) in Lemma 3 hold for $n_i < 6$ and $n_i > 6$, respectively, and that for $n_i = 6$ the equality (18) is obeyed. In the case $n_i = 6$ we may apply Lemma 5. Based on these results and using Lemma 3 we can state

Theorem 8a. *Let G be a hexagonal system with h hexagons, $h \geq 2$, and n_i internal vertices. If $n_i \leq 5$, then Eq. (13) holds for near-zero values of λ. If $n_i \geq 6$ then Eq. (14) holds for near-zero values of λ.*

In a hexagonal system any two vertices whose distance is maximal have degrees equal to 2. Therefore for any hexagonal system G whose diameter is D,

$$(\delta + \Delta)\,\texttt{coeff}_D(H) = 5\,d(G, D) > 4\,d(G, D) = \texttt{coeff}_D(H_1)\ .$$

Applying Lemma 4 we obtain

Theorem 8b. *For all hexagonal systems, Eq. (13) holds for sufficiently large values of λ.*

6. *A Class of Graphs with Large Number of Edges*

Let K_n be the complete graph on n vertices, and let $e_1, e_2, \ldots, e_k$ be independent edges of K_n. Let $K_n(k) \cong K_n - e_1 - e_2 - \cdots - e_k$.

Lemma 9. *Let $n \geq 3$ and $1 \leq k < n/2$. For the graph $G_n(k)$ the following holds: (a) If $k < n/4$, then Eq. (14) holds for near-zero values of λ, there is a positive critical value, and Eq. (13) holds for sufficiently large λ. (b) If $k = n/4$, then there are two critical values: zero and 1. Eq. (14) holds for $0 < \lambda < 1$ and Eq. (13) holds for $\lambda > 1$. (c) If $k > 4n$, then Eq. (13) holds for all non-negative values of λ.*

P r o o f. Lemma 9 follows by direct calculation from

$$H(G_n(k), \lambda) = n + \left[\frac{n(n-1)}{2} - k\right] \lambda + k\,\lambda^2$$

$$H_1(G_n(k),\lambda)=4\left[\frac{n(n-1)}{2}-k\right]+\Big[n(n-1)^2-2k(2n-3)\Big]\,\lambda+2k(n-2)\,\lambda^2$$

by taking into account that $\delta = n-2$, $\Delta = n-1$. □

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