

Mathematical results on harmonic polynomials

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Abstract: The harmonic polynomial was defined in order to understand better the harmonic topological index. Here, we obtain several properties of this polynomial, and we prove that several properties of a graph can be deduced from its harmonic polynomial. Also, we prove that graphs with the same harmonic polynomial share many properties although they are not necessarily isomorphic.

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1. Introduction

A topological descriptor is a real number that depicts a molecule in terms of graph-theoretical elements. Topological descriptors have been widely used on mathematical chemistry studies. A topological index is a topological descriptor that is well correlated with some molecular property. Since the work of Wiener [26] during the middle of the last century, many topological indices have been studied in depth.

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Topological indices are used in various fields, including chemistry, physics, computer science, and network analysis, to analyze and predict properties of molecules, materials, networks, and other systems represented by graphs. Also, they try to capture different aspects of graph structure. Each index provides specific information about the graph and can be used to study and compare graphs, predict properties, or solve optimization problems.

A long list of topological indices has been recognized to be useful in chemical research. Perhaps the Randić index (R) defined in [20] is the best known descriptor (see, e.g., [11, 17, 18, 21, 23] and the references therein). Scientists have been trying to improve the predictive power of Randić's index for years. This race leads to introduce several topological indices, as the first and second Zagreb indices, defined by

$$M_1(\Lambda) = \sum_{uv \in E(\Lambda)} (d_u + d_v) = \sum_{u \in V(\Lambda)} d_u^2, \quad M_2(\Lambda) = \sum_{uv \in E(\Lambda)} d_u d_v,$$

with $E(\Lambda)$ is the set of edges of Λ , the edge uv joins u and v , and d_u is the number of neighbors of u . The interest in the Zagreb's indices has grown and attracted to the scientific community [1, 2, 10, 19, 25].

Another remarkable descriptor is the *harmonic* index [6]:

$$H(\Lambda) = \sum_{uv \in E(\Lambda)} \frac{2}{d_u + d_v}.$$

For more information on the harmonic index see, e.g., [3, 8, 22, 27, 30]. In [31] is introduced the *general sum-connectivity index*, defined as

$$\chi_\alpha(\Lambda) = \sum_{uv \in E(\Lambda)} (d_u + d_v)^\alpha,$$

where α is a real number.

Then, we have that first Zagreb index M_1 is χ_1 , harmonic index H is $2\chi_{-1}$ and sum-connectivity index is $\chi_{-1/2}$. Mathematical properties of this general index were studied in [4, 22, 30–32].

The *harmonic polynomial* with variable x , appears in [16]:

$$A(\Lambda, x) := \sum_{uv \in E(\Lambda)} x^{d_u + d_v - 1},$$

and the harmonic polynomial of some classes of graphs were computed as well. The harmonic polynomials of some line graphs appear in [29]. The harmonic index of many products of graphs are studied in [14] through their harmonic polynomials.

The name of this polynomial comes from the fact that $H(\Lambda) = 2 \int_0^1 A(\Lambda, x) dx$.

Hence, the harmonic polynomial of a graph is a polynomial function that encodes information about the graph structure and the harmonic index. The study of harmonic polynomials in graph theory is aimed at understanding many properties of graphs.

These polynomials can be used to derive bounds on the harmonic index and provide insights into the structural characteristics of graphs.

If Λ_1, Λ_2 are disjoint graphs, we have

$$A(\Lambda_1 \cup \Lambda_2, x) = A(\Lambda_1, x) + A(\Lambda_2, x).$$

Hence, considering connected graphs is not a restrictive condition.

An important problem is to find a polynomial related to a graph that characterizes all graphs, i.e., find a polynomial $P(\Lambda; \cdot)$ such that if $P(\Lambda_1, x) = P(\Lambda_2, x)$, then Λ_1 and Λ_2 are isomorphic graphs. There are several recent articles on the potential of graph polynomials to characterize some types of graphs [24]. Research on the characterization of graphs has been boosted thanks to today's computer power: representing a graph by a polynomial (a vector a low dimension $O(n)$) is simpler than by its adjacency matrix (an $n \times n$ matrix). Several polynomials related to a graph have been defined so far, many of them associated to a graph parameter or to the solution of a graph problem. Some of those polynomials enclose diverse information about the graph's structure. Unfortunately, the problem of characterizing any graph has not been solved by the well-known polynomials yet, since we can often find non-isomorphic graphs having the same polynomial.

In this paper, $\Lambda = (V(\Lambda), E(\Lambda))$ is an unoriented simple graph with minimum degree at least 1. In this paper we study the harmonic polynomial mainly to obtain new properties on this graph polynomial. We prove that several properties of graphs can be obtained from their harmonic polynomials: Corollary 2 characterizes regular and biregular graphs in terms of the zeros of their harmonic polynomials; Theorem 2 gives information about the connectedness, the diameter and the girth (the minimum length of the cycles) of a graph in terms of its harmonic polynomial; Proposition 11 shows that the number of pendant paths is precisely the coefficient of x^2 in the harmonic polynomial. Besides, Theorems 4, 5 and 6 relate the degree sequence of a polynomial with the number of non-zero coefficients of its harmonic polynomial. Theorem 8 shows that graphs with the same harmonic polynomial share interesting properties although they are not necessarily isomorphic.

2. Main Results

In [16] the following result is proved.

Let us recall that the number of vertices (respectively, edges) of a graph is its *order* (respectively, *size*).

Proposition 1. *For every regular graph with degree k and size m ,*

$$A(\Lambda, x) = mx^{2k-1}.$$

The following result is a combination of Propositions 2, 4, 5, 7 in [16] where P_n, C_n, K_n and W_n , respectively, denote the path, the cycle, the complete and the wheel

graphs with order n , respectively, Q_n denotes the n -hypercube, and K_{n_1, n_2} denotes the complete bipartite graph with parts of n_1, n_2 vertices, respectively.

Proposition 2. *For these families of graphs it holds:*

$$\begin{aligned} A(K_n, x) &= \frac{1}{2} n(n-1)x^{2n-3}, \\ A(C_n, x) &= nx^3, \\ A(Q_n, x) &= n2^{n-1}x^{2n-1}, \\ A(K_{n_1, n_2}, x) &= n_1n_2x^{n_1+n_2-1}, \\ A(P_n, x) &= 2x^2 + (n-3)x^3, \\ A(W_n, x) &= (n-1)(x^{n+1} + x^5). \end{aligned}$$

The *forgotten index* was introduced with the Zagreb indices by

$$F(\Lambda) = \sum_{uv \in E(\Lambda)} (d_u^2 + d_v^2) = \sum_{u \in V(\Lambda)} d_u^3.$$

In [13], are defined the formulas for π -electron energy, where the first Zagreb and the forgotten topological indices play an active role. The forgotten index gained attention when [9] shows that this index has a very similar predictive ability to the first Zagreb index. The correlation coefficients shown by both of them were greater than 0.95. Our first result shows that we can relate some properties of the graph with the values of the harmonic polynomial (and its derivatives) at the point 1.

Proposition 3. *For every graph Λ of order n , size m , minimum degree δ and maximum degree Δ , we have:*

- $A(\Lambda, 1) = m$,
- $A'(\Lambda, 1) + A(\Lambda, 1) = M_1(\Lambda)$,
- $A''(\Lambda, 1) - 2A(\Lambda, 1) = F(\Lambda) + 2M_2(\Lambda) - 3M_1(\Lambda)$,
- $A''(\Lambda, 1) + 2A(\Lambda, 1) = M_1(\mathcal{L}(\Lambda)) + M_1(\Lambda)$, where $\mathcal{L}(\Lambda)$ denotes the line graph of Λ .
- $2A(\Lambda, 1)/\Delta \leq n \leq 2A(\Lambda, 1)/\delta$.

Proof. Note that $A(\Lambda, 1) = \sum_{uv \in E(\Lambda)} 1 = m$. Also,

$$A'(\Lambda, 1) = \sum_{uv \in E(\Lambda)} (d_u + d_v) - \sum_{uv \in E(\Lambda)} 1 = M_1(\Lambda) - A(\Lambda, 1),$$

and

$$\begin{aligned}
 A''(\Lambda, 1) &= \sum_{uv \in E(\Lambda)} (d_u^2 + d_v^2) + 2 \sum_{uv \in E(\Lambda)} d_u d_v - 3 \sum_{uv \in E(\Lambda)} (d_u + d_v) + 2 \sum_{uv \in E(\Lambda)} 1 \\
 &= F(\Lambda) + 2M_2(\Lambda) - 3M_1(\Lambda) + 2A(\Lambda, 1), \\
 A''(\Lambda, 1) &= \sum_{uv \in E(\Lambda)} (d_u + d_v - 2)^2 + \sum_{uv \in E(\Lambda)} (d_u + d_v - 2) \\
 &= \sum_{uv \in E(\Lambda)} (d_u + d_v - 2)^2 + \sum_{uv \in E(\Lambda)} (d_u + d_v) - 2 \sum_{uv \in E(\Lambda)} 1 \\
 &= M_1(\mathcal{L}(\Lambda)) + M_1(\Lambda) - 2A(\Lambda, 1).
 \end{aligned}$$

The inequalities $\delta n \leq 2m \leq \Delta n$ and the first item imply the fifth one. □

By Proposition 1, we have that every regular graphs with the same degree and the same size share the harmonic polynomial. Hence, a natural question is: How many graphs characterized by the harmonic polynomial are there? The answer of this question looks like to be difficult, but we can partially respond it. Besides, Proposition 3 gives that graphs with distinct sizes have distinct harmonic polynomial. Next result is an interesting consequence of them.

Corollary 1. *Let Λ be a graph and let Γ be a subgraph of Λ with $\Gamma \neq \Lambda$. Then $A(\Gamma, x) \neq A(\Lambda, x)$.*

Theorem 8 shows below that if two graphs share the harmonic polynomial, then the graphs have to be similar, in some sense.

For each natural number k , consider the polynomial

$$Q_k(x) := \prod_{j=1}^k (x - j) = x^k + \sum_{j=0}^{k-1} a_{k,j} x^j.$$

We can compute these coefficients $a_{k,j}$ in a very simple way:

$$a_{k,k-j} = (-1)^j \sum_{1 \leq i_1 < i_2 < \dots < i_j \leq k} i_1 i_2 \dots i_j.$$

In particular, we have $a_{k,k-1} = -\frac{1}{2}(k+1)k$ and $a_{k,0} = (-1)^k k!$.

Proposition 4. *For every graph Λ and any natural number k , we have*

$$A^{(k)}(\Lambda, 1) = \chi_k(\Lambda) + \sum_{j=0}^{k-1} a_{k,j} \chi_j(\Lambda).$$

Proof. The k -th derivative of $A(\Lambda, x)$ can be computed as follows:

$$A^{(k)}(\Lambda, x) = \sum_{uv \in E(\Lambda)} x^{d_u+d_v-k-1} \prod_{j=1}^k (d_u + d_v - j) = \sum_{uv \in E(\Lambda)} Q_k(d_u + d_v) x^{d_u+d_v-k-1},$$

$$\begin{aligned}
 A^{(k)}(\Lambda, 1) &= \sum_{uv \in E(\Lambda)} Q_k(d_u + d_v) = \sum_{uv \in E(\Lambda)} (d_u + d_v)^k + \sum_{j=0}^{k-1} \sum_{uv \in E(\Lambda)} a_{k,j} (d_u + d_v)^j \\
 &= \chi_k(\Lambda) + \sum_{j=0}^{k-1} a_{k,j} \chi_j(\Lambda).
 \end{aligned}$$

□

As usual, if $A(x)$ is a polynomial, we denote by $\text{Deg}_{\max} A(x)$ its degree. Also, $\text{Deg}_{\min} A(x)$ denotes the minimum degree of the monomials of $A(x)$.

Given a graph Λ ,

$$\begin{aligned}
 \text{Deg}_{\max} A(\Lambda, x) &= \max \{d_u + d_v - 1 \mid uv \in E(\Lambda)\}, \\
 \text{Deg}_{\min} A(\Lambda, x) &= \min \{d_u + d_v - 1 \mid uv \in E(\Lambda)\}.
 \end{aligned}$$

A graph is said to be *biregular* if the graph is bipartite and in each independent set the vertices have the same degree. Such a graph is said to be (Δ, δ) -*biregular* if the degrees in each independent set are Δ and δ .

Proposition 5. *For any graph Λ the following facts hold:*

- For every natural number k and $x \geq 0$, the inequality $A^{(k)}(\Lambda, x) \geq 0$ holds,
- $A(\Lambda, x)$ is strictly positive on $(0, \infty)$ and strictly increasing on $[0, \infty)$,
- Λ has a connected component that is not a single edge if and only if $A(\Lambda, x)$ is a strictly convex function on $[0, \infty)$.

Proof. Since all coefficients of $A(\Lambda, x)$ are greater than or equal to 0, the first item holds.

Since $\text{Deg}_{\min} A(\Lambda, x) \geq 2\delta - 1 \geq 1$, we have $A(\Lambda, x) > 0$ and $A'(\Lambda, x) > 0$ for every $x \in (0, \infty)$.

A graph Λ has a connected component that is not a single edge if and only if $d_u + d_v \geq 3$ for some edge $uv \in E(\Lambda)$; this happens if and only if Λ satisfies $\text{Deg}_{\max} A(\Lambda, x) \geq 2$; and this inequality is equivalent to $A''(\Lambda, x) > 0$ on $(0, \infty)$. □

Υ denotes the set of regular and biregular connected graphs. A collection of graphs $\{\Lambda_i\}_{i=1}^k$, such that Λ_i is either Δ_i -regular or (Δ_i, δ_i) -biregular, for each $1 \leq i \leq k$, is *coherent* if $\Lambda_i \subset \Upsilon$ for all $1 \leq i \leq k$, and $\Delta_i + \delta_i = \Delta_j + \delta_j$ for every $1 \leq i, j \leq k$. A graph is said to be *coherent* if its connected components are coherent.

Fix a graph Λ and a vertex v of Λ . The set of all neighbors of v will be denoted by $N(v)$.

Theorem 1. *For any graph Λ , 0 is the unique root of $A(\Lambda, x)$ if and only if Λ is coherent.*

Proof. If Λ is coherent, let us consider the set of its connected components $\{\Lambda_i\}_{i=1}^k$. For each $1 \leq i \leq k$, Λ_i is either a regular or a (Δ_i, δ_i) -biregular graph with m_i edges; hence, $A(\Lambda_i, x) = m_i x^{\Delta_i + \delta_i - 1}$. So, $m = m_1 + \dots + m_k$ is the cardinality of $E(\Lambda)$, $A(\Lambda, x) = mx^{\Delta_1 + \delta_1 - 1}$ and 0 is the unique root of the polynomial $A(\Lambda, x)$.

Suppose that 0 is the unique root of $A(\Lambda, x)$; thus, $A(\Lambda, x) = ax^{b-1}$ for some natural numbers a, b , and $d_u + d_v = b$ for all $uv \in E(\Lambda)$. Let us consider the set of connected components $\{\Lambda_i\}_{i=1}^k$ of Λ such that Λ_i has maximum degree Δ_i and minimum degree δ_i for each $1 \leq i \leq k$. Thus, given a fixed vertex $u \in V(\Lambda_i)$ one gets $d_v = b - d_u$ for every $uv \in E(\Lambda_i)$, and every $v \in N(u)$ has the same degree $b - d_u$. Similarly, if $w \in N(v)$, we obtain $d_w = b - d_v = d_u$. Since Λ_i is a connected graph, Λ_i is either regular (if $\Delta_i = \delta_i$) or biregular (if $\Delta_i \neq \delta_i$), and $\Lambda_i \subset \mathcal{T}$. Since $\Delta_i + \delta_i = b$ for each $1 \leq i \leq k$, we obtain that Λ is coherent. □

The following consequence of Theorem 1 shows that it is possible to characterize regular and biregular graphs according to the zeros of their harmonic polynomials.

Corollary 2. *If Λ is connected, then $x = 0$ is the unique zero of $A(\Lambda, x)$ if and only if Λ is a biregular or regular graph.*

The following result provides inequalities for the harmonic index according to the value of the harmonic polynomial in the point $1/2$.

Proposition 6. *For any graph Λ is a graph,*

$$A(\Lambda) \geq 2A(\Lambda, 1/2),$$

and Λ satisfies the equality if and only if every connected component of Λ is a single edge.

Proof. Hermite-Hadamard’s inequality states that if $\varphi : [0, 1] \rightarrow \mathbb{R}$ is convex, then

$$\varphi(1/2) \leq \int_0^1 \varphi(x) dx, \tag{1}$$

and the inequality is strict if φ is a strictly convex function.

If some connected component of Λ is not a single edge, then Proposition 5 implies that $A(\Lambda, x)$ is strictly convex. Thus, (1) gives the result. If the graph Λ is the union of m single edges, then $H(\Lambda) = m$, $A(\Lambda, x) = mx$, $A(\Lambda, 1/2) = m/2$. Thus, $2A(\Lambda, 1/2) = H(\Lambda)$. □

If Λ is a graph, $v \in V(\Lambda)$ is said to be *dominant* if $N(v) = V(\Lambda) \setminus \{v\}$.

Proposition 7. *If Λ is a graph with order n , minimum degree δ and maximum degree Δ , then:*

- $x = 0$ is a root of $A(\Lambda, x)$ with multiplicity $\text{Deg}_{\min} A(\Lambda, x)$, where $2\delta - 1 \leq \text{Deg}_{\min} A(\Lambda, x) \leq \text{Deg}_{\max} A(\Lambda, x) \leq 2\Delta - 1$.

- $\text{Deg}_{\max}A(\Lambda, x) \leq 2n - 3$, and $\text{Deg}_{\max}A(\Lambda, x) = 2n - 3$ if and only if there are two adjacent dominant vertices in Λ .
- Let Λ be a graph and Γ a subgraph. Then

$$\text{Deg}_{\max}A(\Gamma, x) \leq \text{Deg}_{\max}A(\Lambda, x), \quad \text{Deg}_{\min}A(\Gamma, x) \leq \text{Deg}_{\min}A(\Lambda, x).$$

Proof. Since

$$A(\Lambda, x) = \sum_{j=\text{Deg}_{\min}A(\Lambda, x)}^{\text{Deg}_{\max}A(\Lambda, x)} c_j x^j,$$

for some constants c_j , 0 is a root of the polynomial $A(\Lambda, x)$ with multiplicity $\text{Deg}_{\min}A(\Lambda, x)$. Since each j in the previous sum can be written as $d_u + d_v - 1$ for a $uv \in E(\Lambda)$, we have $2\delta - 1 \leq \text{Deg}_{\min}A(\Lambda, x) \leq \text{Deg}_{\max}A(\Lambda, x) \leq 2\Delta - 1$.

Since $\Delta \leq n - 1$, we have $\text{Deg}_{\max}A(\Lambda, x) \leq 2n - 3$. Therefore, $\text{Deg}_{\max}A(\Lambda, x) = 2n - 3$ if and only if there is $uv \in E(\Lambda)$ with $d_u = d_v = n - 1$, and this happens if and only if u, v are dominant vertices in the graph Λ .

Let Γ be a subgraph of Λ . The last statement holds, since the degree of $v \in \Gamma$ is at most its degree in Λ . □

Recall that the minimum length of the cycles in a graph is its *girth*. The following result gives some relations involving the order, diameter, connectivity, girth of a graph, and the degree of its harmonic polynomial.

Theorem 2. *Consider any graph Λ with order n . If $\text{Deg}_{\max}A(\Lambda, x) \geq n$, then $g(\Lambda) = 3$. Furthermore, if Λ is triangle-free and $\text{Deg}_{\max}A(\Lambda, x) = n - 1$, then Λ is connected and $\text{diam}\Lambda \leq 3$.*

Proof. Since $g(\Lambda) = 3$ if and only if Λ is not triangle-free, it suffices to prove that if Λ is triangle-free, then $\text{Deg}_{\max}A(\Lambda, x) \leq n - 1$. Since Λ is triangle-free, then $N(u) \cap N(v) = \emptyset$ for any $uv \in E(\Lambda)$. Hence, $d_u + d_v \leq n$ for any $uv \in E(\Lambda)$, and $\text{Deg}_{\max}A(\Lambda, x) \leq n - 1$.

Assume that Λ is triangle-free and $\text{Deg}_{\max}A(\Lambda, x) = n - 1$. Thus, there is an edge $uv \in E(\Lambda)$ with $d_u + d_v = n$. Since $N(u) \cap N(v) = \emptyset$, we have $N(u) \cup N(v) = V(\Lambda)$ and $d(w, \{u, v\}) \leq 1$ for every $w \in V(\Lambda)$. Consequently, $\text{diam}\Lambda \leq 3$ and Λ is connected. □

If $A(x)$ is a polynomial, $K(A(x))$ denotes the number of its coefficients that are non-zero.

Theorem 3. *If Λ is a graph with size m , then:*

- $1 \leq K(A(\Lambda, x)) \leq m$,
- $K(A(\Lambda, x)) = 1$ if and only if Λ is coherent,
- $K(A(\Lambda, x)) = m$ if and only if Λ is a single edge.

Proof. The first item is straightforward.

The proof of Theorem 1 implies that Λ is coherent if and only if $A(\Lambda, x) = ax^{b-1}$ for some natural numbers a, b , and this is equivalent to $K(A(\Lambda, x)) = 1$.

If Λ is a single edge, then it is regular graph, and the previous item gives $K(A(\Lambda, x)) = 1 = m$.

If Λ is not a single edge, then we consider several cases.

(1) Λ is connected. Thus, $3 \leq d_u + d_v \leq m + 1$ for any $uv \in E(\Lambda)$, i.e., $2 \leq d_u + d_v - 1 \leq m$. Since the m values of $d_u + d_v - 1$ belong to a set of $m - 1$ integers, there are two edges with the same value and we conclude that $K(A(\Lambda, x)) \leq m - 1$.

(2) If Λ has connected components $\Lambda_1, \dots, \Lambda_k$, with $k \geq 2$, denote by m_i the cardinality of the edges of Λ_i ; thus, $m = m_1 + \dots + m_k$.

(2.1) Assume that there exists some $1 \leq j \leq k$ such that Λ_i is not isomorphic to P_2 . So, (1) gives that $K(A(\Lambda_j, x)) \leq m_j - 1$, and this inequality and the first item give

$$K(A(\Lambda, x)) \leq \sum_{i=1}^k K(A(\Lambda_i, x)) \leq \sum_{i=1}^k m_i - 1 = m - 1.$$

(2.2) Assume that Λ_i is isomorphic to P_2 for every $1 \leq i \leq k$. So, $m = k \geq 2$,

$$A(\Lambda, x) = \sum_{i=1}^m A(\Lambda_i, x) = \sum_{i=1}^m x = mx,$$

and $K(A(\Lambda, x)) = 1 \leq k - 1 < m$. □

Theorem 3 has the following corollary.

Corollary 3. *If Λ is a graph with order $m \geq 2$, then $1 \leq K(A(\Lambda, x)) \leq m - 1$.*

Proposition 8. *Let Λ be a graph with size m , order n , maximum degree Δ and minimum degree δ . Then:*

- $K(A(\Lambda, x)) \leq \text{Deg}_{\max} A(\Lambda, x) - \text{Deg}_{\min} A(\Lambda, x) + 1$.
- $K(A(\Lambda, x)) \leq \min\{2\Delta - 2\uparrow 1, m - 2\uparrow 2\}$.
- *If Λ is triangle-free, then $K(A(\Lambda, x)) \leq n - 2\uparrow 1$.*

Proof. The first item holds since there are constants c_j with

$$A(\Lambda, x) = \sum_{j=\text{Deg}_{\min} A(\Lambda, x)}^{\text{Deg}_{\max} A(\Lambda, x)} c_j x^j,$$

The first item and the bounds in Proposition 7 give $K(A(\Lambda, x)) \leq 2\Delta - 2\uparrow 1$. Since $d_u + d_v - 1 \leq m$ for any $uv \in E(\Lambda)$, we have $\text{Deg}_{\max} A(\Lambda, x) \leq m$. This inequality, the first item and the first item in Proposition 7 give $K(A(\Lambda, x)) \leq m - 2\uparrow 2$.

The third item is a consequence of the first one, the first item in Proposition 7 and Theorem 2. □

If Λ is a graph, $DS(\Lambda) = \{d_u\}_{u \in V(\Lambda)}$ is the *degree sequence* of Λ (if $d_{v_1} = d_{v_2}$ for some $v_1, v_2 \in V(\Lambda)$, then the value $d_{v_1} = d_{v_2}$ appears just once in $\{d_u\}_{u \in V(\Lambda)}$).

Let us denote by $\lceil t \rceil$ the upper integer part of $t \in \mathbb{R}$, i.e., the smallest integer greater than or equal to t .

Theorem 4. *If Λ is any graph, then:*

- If $DS(\Lambda)$ has at most r terms, then $K(A(\Lambda, x)) \leq \frac{r(r+1)}{2}$.
- If $K(A(\Lambda, x)) \geq s$, then $DS(\Lambda)$ has at least $\lceil \frac{\sqrt{8s+1}-1}{2} \rceil$ terms.

Proof. If $DS(\Lambda)$ has at most r terms, then the set of different values $d_u + d_v$ has cardinality at most $r(r+1)/2$ (2-combinations with repetition of a set of r elements). Thus, $K(A(\Lambda, x)) \leq r(r+1)/2$.

Assume that $K(A(\Lambda, x)) = S \geq s$, and denote by r the cardinality of $DS(\Lambda)$. The first item gives

$$s \leq S \leq \frac{r(r+1)}{2}, \quad r^2 + r - 2s \geq 0, \quad r \geq \frac{\sqrt{8s+1}-1}{2},$$

and we obtain the desired inequality since r is an integer. □

One can think that it might be possible to obtain a lower bound for $K(A(\Lambda, x))$ that is an increasing function of the cardinality of $DS(\Lambda)$. However, next theorem shows that this is not possible.

Theorem 5. *Let Λ be a connected graph with r terms in $DS(\Lambda)$.*

- If $r \leq 2$, then $K(A(\Lambda, x)) \geq 1$.
- If $r > 2$, then $K(A(\Lambda, x)) \geq 2$.

Furthermore, the bounds are sharp for each r .

Proof. The first statement follows from Theorem 3.

Assume now that $r > 2$. Since Λ is connected, there exist a path $\gamma = \{u_1, u_2, \dots, u_k\}$ in Λ and three vertices in $V(\Lambda) \cap \gamma$ with different degrees. One can assume that

$$d_{u_1} \notin \{d_{u_2}, \dots, d_{u_k}\} \quad \text{and} \quad d_{u_k} \notin \{d_{u_1}, \dots, d_{u_{k-1}}\},$$

since otherwise u_1 and/or u_k can be removed from γ , and a shorter path with the same property is obtained. Also, we can assume that $d_{u_2} = d_{u_3} = \dots = d_{u_{k-2}} = d_{u_{k-1}}$. Thus, $d_{u_1} + d_{u_2} \neq d_{u_2} + d_{u_k} = d_{u_{k-1}} + d_{u_k}$ and, since $u_1u_2, u_{k-1}u_k \in E(\Lambda)$, we conclude $K(A(\Lambda, x)) \geq 2$.

If Λ is a star graph of order n , then $DS(\Lambda) = \{1, n - 1\}$; thus $r = 1$ if $n = 2$, and $r = 2$ if $n > 2$. Since $A(\Lambda, x) = (n - 1)x^{n-1}$, we have $K(A(\Lambda, x)) = 1$.

Consider the sequence $\{1, 2, \dots, r\}$ with $r > 2$. We are going to define a graph T_r (in fact, T_r is a tree) with $DS(\Lambda) = \{1, 2, \dots, r\}$ and $K(A(T_r, x)) = 2$. Let us consider the (ordered) sequence $\{a_1, a_2, \dots, a_r\}$ obtained as a permutation of $\{1, 2, \dots, r\}$ in the following way. If r is even, then

$$\{a_1, a_2, \dots, a_r\} = \left\{ \frac{r}{2} + 1, \frac{r}{2}, \frac{r}{2} + 2, \frac{r}{2} - 1, \dots, r - 1, 2, r, 1 \right\}.$$

If r is odd, then

$$\{a_1, a_2, \dots, a_r\} = \left\{ \frac{r+1}{2}, \frac{r+1}{2} + 1, \frac{r+1}{2} - 1, \frac{r+1}{2} + 2, \frac{r+1}{2} - 2, \dots, r - 1, 2, r, 1 \right\}.$$

In both cases we have that $a_j + a_{j+1}$ is either $r + 1$ or $r + 2$ for each $1 \leq j < r$. Consider a point v_1 , which will be the root of T_r . We define T_r inductively on the distance j from v_1 . We join v_1 with a_1 vertices (at distance 1 from v_1). If $u \in V(T_r)$ with $d_{T_r}(u, v_1) = j - 1$ for some $1 < j < r$, then we join u with $a_j - 1$ vertices (at distance j from v_1). Note that if $u \in V(T_r)$, then $d_{T_r}(u, v_1) = j - 1$ for some $1 \leq j < r$ and $d_u = a_j$. If $uv \in E(T_r)$, then one can assume that there exists $1 \leq j < r$ with $d_{T_r}(u, v_1) = j - 1$ and $d_{T_r}(v, v_1) = j$. Therefore, $d_u + d_v = a_j + a_{j+1}$ is either $r + 1$ or $r + 2$, and so $K(A(T_r, x)) = 2$. □

Theorem 6. *Let Λ be a graph.*

- *If some connected component of Λ has a degree sequence of cardinality $r > 2$, then $K(A(\Lambda, x)) \geq 2$.*
- *For each $r \geq 1$, there exists Λ with $SD(\Lambda)$ of cardinality r and $K(A(\Lambda, x)) = 1$.*

Proof. If there is a connected component Λ_i of Λ with degree sequence of cardinality $r > 2$, then Theorem 5 gives $K(A(\Lambda_i, x)) \geq 2$, and $K(A(\Lambda, x)) \geq K(A(\Lambda_i, x)) \geq 2$.

Fix any $r \geq 1$.

If r is even, then define Λ_r as the union of the complete bipartite graphs

$$K_{1,r}, K_{2,r-1}, \dots, K_{r/2-1,r/2+2}, K_{r/2,r/2+1}.$$

If r is odd, then define Λ_r as the union of

$$K_{1,r}, K_{2,r-1}, \dots, K_{(r+1)/2-1,(r+1)/2+1}, K_{(r+1)/2,(r+1)/2}.$$

In both cases, the degree sequence of Λ_r has cardinality r . If m denotes the cardinality of $E(\Lambda_r)$, then $A(\Lambda_r, x) = mx^r$ and $K(A(\Lambda_r, x)) = 1$. □

We say that $DS(\Lambda)$ is even (respectively, odd) if $DS(\Lambda) = \{d_u\}_{u \in V(\Lambda)}$ is contained the even (respectively, odd) integers.

Proposition 9. *For any graph Λ , $A(\Lambda, x)$ is an odd function if and only if the degree sequence of each connected component of Λ is either even or odd.*

Proof. If the degree sequence of each connected component of Λ is either even or odd, then $d_u + d_v - 1$ is odd for any $uv \in E(\Lambda)$. Since every exponent in $A(\Lambda, x)$ is odd, $A(\Lambda, x)$ is an odd function.

Assume now that $A(\Lambda, x)$ is odd. Therefore, $d_u + d_v$ is even for every $uv \in E(\Lambda)$. Consider any fixed connected component Λ_i of Λ . If there is $u \in V(\Lambda_i)$ such that d_u is even, then d_v is even for any $v \in N(u)$. Since Λ_i is connected, we conclude that the degree sequence of Λ_i is even. The same argument gives that if there is $u \in V(\Lambda_i)$ with d_u odd, the degree sequence of Λ_i is odd. \square

We say that Λ has *alternated degree* if d_u and d_v have different oddity for any $u, v \in V(\Lambda)$ with $uv \in E(\Lambda)$.

From the above definition, the following result is obtained.

Proposition 10. *For any graph Λ , $A(\Lambda, x)$ is an even function if and only if Λ has alternated degree.*

An edge is *pendant* if one of its vertices has degree 1. A path with length two is a *pendant path* if it contains a pendant edge and a non-pendant edge.

Proposition 11. *For any graph Λ , the cardinality of the pendant paths in Λ is the coefficient of x^2 in $A(\Lambda, x)$.*

Proof. There exists a bijective map between the pendant paths in Λ and the edges $uv \in E(\Lambda)$ with $d_u = 1$ and $d_v = 2$ (i.e., $d_u + d_v - 1 = 2$). This gives the result. \square

There are inequalities relating the harmonic index and the first Zagreb index ([15], [28, Theorem 2.5], [12, p.234]). One of these results can be stated as:

Theorem 7. *If Λ is a graph with minimum degree δ , maximum degree Δ and size m , then*

$$\frac{2m^2}{M_1(\Lambda)} \leq H(\Lambda) \leq \frac{(\Delta + \delta)^2 m^2}{2\Delta\delta M_1(\Lambda)}.$$

In 2009, Fath-Tabar [7] defined the first Zagreb polynomial as

$$M_1(\Lambda, x) := \sum_{uv \in E(\Lambda)} x^{d_u + d_v}.$$

Theorem 7 relates the first Zagreb and the harmonic indices. Notice that there is a direct relation between definitions of the harmonic polynomial and the first Zagreb polynomial, i.e., $M_1(\Lambda, x) = x A(\Lambda, x)$. The following proposition provides new bounds for $\text{Deg}_{\min} A(\Lambda, x)$ and $\text{Deg}_{\max} A(\Lambda, x)$.

Proposition 12. *If Λ is a graph with size m , order n , maximum degree Δ and minimum degree δ , then*

$$2 \cdot 1 \leq \text{Deg}_{\min} A(\Lambda, x) \leq \frac{A'(\Lambda, 1)}{m}, \quad \frac{4m}{n} - 1 \leq \text{Deg}_{\max} A(\Lambda, x) \leq 2\Delta - 1.$$

Proof. The inequality $A(\Lambda) \leq n/2$ is a well-known upper bound for the harmonic index. Theorem 7 gives the lower bound $A(\Lambda) \geq 2m^2/M_1(\Lambda)$. Given $j \in \mathbb{N}$, define $c_j = c_j(\Lambda)$ as the cardinality of the set $\{uv \in E(\Lambda) \mid d_u + d_v = j + 1\}$. One can write

$$A(\Lambda, x) = \sum_{j=\text{Deg}_{\min} A(\Lambda, x)}^{\text{Deg}_{\max} A(\Lambda, x)} c_j x^j, \quad \text{with} \quad \sum_{j=\text{Deg}_{\min} A(\Lambda, x)}^{\text{Deg}_{\max} A(\Lambda, x)} c_j = m.$$

Thus, we have

$$\begin{aligned} \frac{n}{2} &\geq H(\Lambda) = 2 \int_0^1 A(\Lambda, x) dx = \sum_{j=\text{Deg}_{\min} A(\Lambda, x)}^{\text{Deg}_{\max} A(\Lambda, x)} \frac{2c_j}{j+1} \\ &\geq \sum_{j=\text{Deg}_{\min} A(\Lambda, x)}^{\text{Deg}_{\max} A(\Lambda, x)} \frac{2c_j}{\text{Deg}_{\max} A(\Lambda, x) + 1} = \frac{2m}{\text{Deg}_{\max} A(\Lambda, x) + 1}, \\ \text{Deg}_{\max} A(\Lambda, x) &\geq \frac{4m}{n} - 1, \\ \frac{2m^2}{M_1(\Lambda)} &\leq H(\Lambda) = \sum_{j=\text{Deg}_{\min} A(\Lambda, x)}^{\text{Deg}_{\max} A(\Lambda, x)} \frac{2c_j}{j+1} \leq \frac{2m}{\text{Deg}_{\min} A(\Lambda, x) + 1}, \\ \text{Deg}_{\min} A(\Lambda, x) &\leq \frac{M_1(\Lambda)}{m} - 1 = \frac{M_1(\Lambda) - m}{m} = \frac{A'(\Lambda, 1)}{m}. \end{aligned}$$

Proposition 7 provides the other inequalities. □

The next result allows to bound the harmonic index in terms of several parameters of its harmonic polynomial.

If Λ is a graph, denote by $c_{\min}(\Lambda)$ and $c_{\max}(\Lambda)$ the coefficients of $x^{\text{Deg}_{\min} A(\Lambda, x)}$ and $x^{\text{Deg}_{\max} A(\Lambda, x)}$ in $A(\Lambda, x)$, respectively.

Proposition 13. *If Λ be a graph with size m , then*

$$\frac{2c_{\min}(\Lambda)}{\text{Deg}_{\min} A(\Lambda, x) + 1} + \frac{2m - 2c_{\min}(\Lambda)}{\text{Deg}_{\max} A(\Lambda, x) + 1} \leq A(\Lambda) \leq \frac{2c_{\max}(\Lambda)}{\text{Deg}_{\max} A(\Lambda, x) + 1} + \frac{2m - 2c_{\max}(\Lambda)}{\text{Deg}_{\min} A(\Lambda, x) + 1}.$$

Proof. As in the proof of Proposition 12, we obtain

$$H(\Lambda) = 2 \int_0^1 A(\Lambda, x) dx = \sum_{j=\text{Deg}_{\min} A(\Lambda, x)}^{\text{Deg}_{\max} A(\Lambda, x)} \frac{2c_j}{j+1}.$$

Hence,

$$\begin{aligned}
 H(\Lambda) &= \frac{2c_{\min}(\Lambda)}{\text{Deg}_{\min} A(\Lambda, x) + 1} + \sum_{j=\text{Deg}_{\min} A(\Lambda, x)+1}^{\text{Deg}_{\max} A(\Lambda, x)} \frac{2c_j}{j+1} \\
 &\geq \frac{2c_{\min}(\Lambda)}{\text{Deg}_{\min} A(\Lambda, x) + 1} + \sum_{j=\text{Deg}_{\min} A(\Lambda, x)+1}^{\text{Deg}_{\max} A(\Lambda, x)} \frac{2c_j}{\text{Deg}_{\max} A(\Lambda, x) + 1} \\
 &= \frac{2c_{\min}(\Lambda)}{\text{Deg}_{\min} A(\Lambda, x) + 1} + \frac{2m - 2c_{\min}(\Lambda)}{\text{Deg}_{\max} A(\Lambda, x) + 1}, \\
 H(\Lambda) &= \frac{2c_{\max}(\Lambda)}{\text{Deg}_{\max} A(\Lambda, x) + 1} + \sum_{j=\text{Deg}_{\min} A(\Lambda, x)}^{\text{Deg}_{\max} A(\Lambda, x)-1} \frac{2c_j}{j+1} \\
 &\leq \frac{2c_{\max}(\Lambda)}{\text{Deg}_{\max} A(\Lambda, x) + 1} + \sum_{j=\text{Deg}_{\min} A(\Lambda, x)}^{\text{Deg}_{\max} A(\Lambda, x)-1} \frac{2c_j}{\text{Deg}_{\min} A(\Lambda, x) + 1} \\
 &= \frac{2c_{\max}(\Lambda)}{\text{Deg}_{\max} A(\Lambda, x) + 1} + \frac{2m - 2c_{\max}(\Lambda)}{\text{Deg}_{\min} A(\Lambda, x) + 1}.
 \end{aligned}$$

□

Theorem below shows that if two graphs have the same harmonic polynomial, then they share several properties. However, two non-isomorphic graphs could share the harmonic polynomial.

Given function $\mu : \mathbb{N} \rightarrow \mathbb{R}_+$, define its associated topological indices

$$T_\mu(\Lambda) = \sum_{uv \in E(\Lambda)} \mu(d_u + d_v), \quad U_\mu(\Lambda) = \prod_{uv \in E(\Lambda)} \mu(d_u + d_v).$$

In particular, if $\mu(t) = t^\alpha$, then $T_\mu = \chi_\alpha$. The *modified first multiplicative Zagreb index* is $\Pi_1^*(\Lambda) = \prod_{uv \in E(\Lambda)} (d_u + d_v)$, see [5]. In particular, if $\mu(t) = t$, then $U_\mu = \Pi_1^*$.

Theorem 8. *If two graphs Λ_1 and Λ_2 have the same harmonic polynomial, then $T_\mu(\Lambda_1) = T_\mu(\Lambda_2)$ and $U_\mu(\Lambda_1) = U_\mu(\Lambda_2)$ for every function $\mu : \mathbb{N} \rightarrow (0, \infty)$. In particular, $\chi_\alpha(\Lambda_1) = \chi_\alpha(\Lambda_2)$ for every $\alpha \in \mathbb{R}$, and $\Pi_1^*(\Lambda_1) = \Pi_1^*(\Lambda_2)$.*

Proof. As in the proof of Proposition 12, given a graph Λ and $j \in \mathbb{N}$, we define $c_j(\Lambda)$ as the cardinality of $\{uv \in E(\Lambda) \mid d_u + d_v = j + 1\}$. Thus, $A(\Lambda, x) = \sum_j c_j(\Lambda) x^j$. If $A(\Lambda_1, x) = A(\Lambda_2, x)$, then $c_j(\Lambda_1) = c_j(\Lambda_2)$ for every $j \in \mathbb{N}$. Since $T_\mu(\Lambda) = \sum_j c_j(\Lambda) \mu(j + 1)$ and $U_\mu(\Lambda) = \prod_j \mu(j + 1)^{c_j(\Lambda)}$ for every function $\mu : \mathbb{N} \rightarrow (0, \infty)$, we conclude that $T_\mu(\Lambda_1) = T_\mu(\Lambda_2)$ and $U_\mu(\Lambda_1) = U_\mu(\Lambda_2)$. □

We want to remark that if we consider a function $\mu : \mathbb{N} \rightarrow \mathbb{C}$ in the definition T_μ , then the argument in the proof of Theorem 8 also works. Thus, we can consider a family of functions $\{\mu_z\}$, where z is a complex variable, and we can define for each graph Λ the complex function $F_\Lambda(z) := T_{\mu_z}(\Lambda)$. So, if two graphs Λ_1 and Λ_2 have the same harmonic polynomial, then the complex functions $F_{\Lambda_1}(z)$ and $F_{\Lambda_2}(z)$ are the same. This holds, in particular, for the holomorphic function $F_\Lambda(z) := \sum_{uv \in E(\Lambda)} (d_u + d_v)^z$.

Conclusions

In this work, we obtain several properties of the harmonic polynomial and we prove that certain graph properties can be derived from their corresponding associated polynomials. Namely, we characterize regular and biregular graphs by examining the zeros of their harmonic polynomials (Corollary 2). In Theorem 2, we provide insights into the graph's connectivity, diameter, and circumference in relation to the degree of its harmonic polynomial. Proposition 11 demonstrates that the coefficient of x^2 in the harmonic polynomial represents the cardinality of the set of pendant paths in the graph. Furthermore, Theorems 4, 5 and 6 establish a relationship between the number of nonzero coefficients in the harmonic polynomial and the polynomial's degree sequence. Lastly, Theorem 8 establishes that two graphs sharing the same harmonic polynomial must be similar.

There are still some open problems; for example, studying the mathematical properties of other polynomials associated with different indices; as well as studying the harmonic polynomial on graph operators.

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