MATCH
Communications in Mathematical and in Computer Chemistry

*MATCH Commun. Math. Comput. Chem.* **92** (2024) 567–587
**ISSN:** 0340–6253
**doi:** 10.46793/match.92-3.567G

# A Survey on Orbit Polynomials

**Modjtaba Ghorbani**[a,*], **Razie Alidehi–Ravandi**[b], **Matthias Dehmer**[c,d,e]

[a] *Department of Mathematics, Faculty of Science, Shahid Rajaee, Teacher Training University, Tehran, 16785-163, I. R. Iran*
[b] *Department of Computer Science, Swiss Distance University of Applied Sciences, 3900 Brig, Switzerland;*
[c] *Department of Biomedical Computer Science and Mechatronics, Tyrolean private university UMIT TIROL, A-6060 Hall in Tyrol, Austria*
[d] *College of Artficial Intelligence, Nankai University, Tianjin 300071, China*

mghorbani@sru.ac.ir, RazieRavandi@sru.ac.ir, Matthias.Dehmer@umit.at

(Received December 17, 2023)

**Abstract**

In this article, we survey the results on examining orbit structures combined with polynomials, automorphism groups, roots of polynomials, and the construction of graphs with prescribed orbit structures. The orbit polynomial has been defined as the $\sum_n cx^n$, where $c$ represents the number of orbits of graph $G$ with size $n$. By subtracting this polynomial from 1, the modified orbit polynomial $O^{\star}_G(x) = 1 - O_G(x)$ is obtained which possesses a unique positive root denoted by $\delta$. This root can be seen as a relative measure of symmetry. The study of orbit structures in graphs and their associated automorphism groups is a fundamental topic in graph theory. The understanding and analysis of these structures provide valuable insights into the symmetries in graphs, enabling the exploration of various graph properties and their applications in diverse fields such as network analysis, computer science, and chemistry.

*Corresponding author.

# 1 Introduction

In the field of quantum chemistry, the early Hückel theory has been used to calculate the energy levels of $p$-electrons in conjugated hydrocarbons. These energy levels are determined as the eigenvalues of the characteristic/spectral polynomial associated with the molecular graph [4]. Hosoya [20] and other researchers [14, 16, 17] extended this concept by replacing the adjacency matrix with other matrices based on graph invariants.

Counting polynomials in mathematical chemistry were initially introduced by Hosoya [21]. Subsequently, various other counting polynomials were proposed, such as the matching polynomial [7, 15, 19], independence polynomial [13, 18], king polynomial [3, 24], color polynomial [3], and star or clique polynomials [8,9]. A comprehensive overview of graph polynomials can be found in reference [1]. By having the orbits and their structures in a graph, we can infer many algebraic properties about the automorphism group and thus about the similar vertices. For example, the length of orbits of a network provides important information about each individual component in the network. In other words, all vertices in an orbit have the same properties such as the degree of vertices which yield useful data about the number of components' interconnections. Finding the counting polynomial [20] of a graph often helps to investigate the structural properties of regarding graph.

Dehmer et al. [5] introduced the orbit polynomial as a significant polynomial that utilizes vertex orbit sizes' cardinalities. The orbit polynomial is defined as $\sum_n cx^n$, where $c$ represents the number of orbits of graph $G$ with size $n$, and the coefficients are all positive. By subtracting this polynomial from 1, the modified orbit polynomial $O^\star_G(x) = 1 - O_G(x)$ is obtained, which possesses a unique positive root denoted by $\delta$. This root can be utilized as a relative measure of a graph's symmetry and is an indicator of the level of symmetry present, allowing for comparisons between graphs based on this characteristic.

Furthermore, certain bounds for the unique positive root of $O^\star_G$ were computed in [5], demonstrating its significant value in various fields, including chemistry, bioinformatics, and structure-oriented drug design. In

[11], a study explored the structural attributes of a graph's automorphism group, the corresponding orbit polynomial for certain graph operations, and introduced a new counting polynomial for comparison to the degeneracy of an orbit polynomial.

It is important to note that characteristic polynomials do not uniquely characterize graphs due to the existence of isospectral graphs [2].

The study of orbit structures in graphs and their associated automorphism groups is a fundamental topic in graph theory. The understanding and analysis of these structures provide valuable insights into the symmetries present in graphs, allowing for the exploration of various graph properties and their applications in several fields such as crystallography [25], physics [29], network analysis [22], computer science [30], engineering sciences [28] and chemistry [26]. This survey article aims to present a comprehensive overview of the results obtained in the study of orbit structures in graphs. We proceed as follow:

In Section 2, all definitions and results needed in this paper are given. The Section 3 focuses on the results related to orbit polynomials and automorphism groups. These results establish connections between the number of orbits and the structure of the automorphism group of a graph. Theorems such as the edge-orbit polynomial theorem and the relationship between the orbit polynomial and the automorphism group shed light on the nature of these structures and their influence on graph properties. Besides, this section explores the roots of orbit polynomials. Investigating the properties and characteristics of these roots provides valuable information about the symmetries and structures of graphs. Lemmas and theorems related to the uniqueness, bounds, and distribution of these roots offer important tools for analyzing the symmetries present in different types of graphs. In continuing this section, the focus shifts to graphs with three distinct orbit sizes. Theorems and corollaries in this section investigate the properties of such graphs and provide conditions for the existence and behavior of their orbit polynomials. Understanding the symmetries present in graphs with multiple orbit sizes contributes to a deeper comprehension of their overall structure and properties.

Lastly, Section 4 explores the construction and interpretation of graphs that achieve prescribed orbit structures. Theorems and algorithms related to these constructions provide valuable insights into the possibilities of designing graphs with specific orbit structures, allowing for the customization of graph properties for various applications.

Overall, this survey article aims to provide a comprehensive overview of the results obtained in the study of orbit structures in graphs. By exploring the relationships between orbit polynomials, automorphism groups, roots of polynomials, and the construction of graphs with prescribed orbit structures, we gain valuable insights into the symmetries and properties of graphs.

## 2 Preliminaries

In this study, we use the notation $V(G)$ and $E(G)$ to represent the sets of vertices and edges of the graph $G$, respectively. We consider graphs that are finite, simple, and connected.

The automorphism group consists of all permutations on the set of vertices that preserve their adjacency relationship. For a graph $G$, $e = xy$ is an edge if and only if $p(x)p(y)$ is an edge. We denote the automorphism group of graph $G$ by $Aut(G)$.

A vertex orbit for a vertex $u$ in graph $G$ is the set of all images $\alpha(v)$, where $\alpha$ is an automorphism of $G$. If a graph $G$ is vertex-transitive, it means that it has only one orbit and thus all vertices are interchangeable. A similar concept applies to edge-transitive graphs.

Next, we consider an edge-automorphism of a graph $G$, which is a bijection on the set of edges that maintains adjacency. The set of all edge-automorphisms of a graph $G$ forms a group under the composition of functions. An automorphism of $G$ gives rise to a corresponding edge-automorphism of $G$. The set $Aut^\star(G)$ is a subgroup of $Aut(G)$ containing edge-automorphisms of $G$ induced by each automorphism of $G$.

Given the method of action of the automorphism group of graph $G$ on the edge set, we can define the edge orbit polynomial as follows.

**Definition 1.** Suppose $E_1, \ldots, E_h$ are all edge-orbits under the action of the group $Aut(G)$ on the edge set of $G$. We define the edge-orbit polynomial of $G$ as:

$$\bar{O}_G(x) = \sum_{i=1}^{h} x^{|E_i|}.$$

Moreover, we can define the modified version of the edge orbit polynomial as:

$$\bar{O}^{\star}_G(x) = 1 - \sum_{i=1}^{h} x^{|E_i|}.$$

Here, $|E_i|$ signifies the number of edges in the $i$-th edge orbit of $G$ under the action of $Aut(G)$.

We define the support of an automorphism $g \in Aut(G)$ as $supp(g) = \{g(u) : u \in V(G)\}$. Two permutations $f$ and $g$ are said to be disjoint if $supp(f) \cap supp(g) = \emptyset$. Let $A$ and $B$ be finite groups and $B$ act on the set $X$. The wreath product of groups $A$ and $B$ is a group given by:

$$A \wr B = \{(f, b) \mid f : X \to A \text{ is a function, } b \in B\}.$$

We can define the group operation as $(f_1, b_1)(f_2, b_2) = (g, b_1b_2)$, where for any $i \in X$, $g(i) = f_1(i)f_2(i^{b_1})$. The wreath product is useful in describing the symmetry of networks. For example, let $H$ be a network formed from the union of $r$ copies of a graph $M$. Then, we have $Aut(H) \cong S_r \wr Aut(M)$, which means that the automorphisms of $H$ consist of permutations of the copies of $M$ that commute with $Aut(M)$, together with permutations of the copies induced by $Aut(M)$.

# 3 Results

In summary, this section explores various aspects of orbit polynomials and their relation to graph symmetry. It presents several theorems and results that provide insights into the properties of graphs with multiple orbit sizes. The section also discusses the use of the measure $\delta$ as a relative indicator of graph symmetry and its correlation with other symmetry measures. Furthermore, it introduces a method for constructing graphs with prescribed orbit structures, which offers a valuable tool for generating graphs with a well-defined degree of symmetry. These results contribute to our understanding of graph symmetry and provide new perspectives on the relationship between algebraic and information-theoretic measures.

## 3.1 Orbit polynomials and automorphism groups

Here, we report various theorems and corollaries related to orbit polynomials and automorphism groups. We begin with the theorem stated in [10], which implies that for a network $\mathcal{N}$ with $n$ vertices and $(n-1)$ orbits, the orbit polynomial $O_{\mathcal{N}}$ is given by $O_{\mathcal{N}}(x) = x^2 + (n-2)x$, and the automorphism group $Aut(\mathcal{N})$ is isomorphic to $\mathbb{Z}_2$. This theorem provides valuable information about the orbit polynomial and automorphism group of networks with a specific number of vertices and orbits.

Next, we explore another theorem from [11] that relates the edge-orbit polynomial $\bar{O}_T(x)$ to the graph isomorphism with $S_n$. Moving on, we encounter a theorem from [11] that focuses on graphs without pendant edges. The theorem states that if the orbit polynomial $O_G$ is equal to $\bar{O}_G$, then $G$ is isomorphic to the cycle graph $C_n$. This result highlights the relationship between the orbit polynomial and the graph structure, specifically for graphs without pendant edges.

Additionally, we come across a theorem from [12] that examines the orbit polynomial $O_G$ of a graph $G$ with order $n$ and coefficients $a$, $b$, and $c$. The theorem implies that if $1 \leq a, b, c \leq 3$, then the automorphism group $Aut(G)$ is a $\{2,3\}$-group. This theorem provides insights into the automorphism group structure based on the coefficients of the orbit polynomial.

Furthermore, we discuss a corollary from [22] that builds upon the concept of generators and support sets of the automorphism group. The corollary establishes the relationship between the orbit polynomial $O_G$ and the support sets of the generators.

To illustrate the concepts discussed, we consider a specific graph $G$ depicted in Figure 1. The graph exhibits a typical arrangement of symmetric subgraphs found in real-world networks. The authors in [22] determined the automorphism group structure of $G$ as $Aut(G) \cong \mathbb{Z}_2^2 \times S_3 \times S_4 \times (\mathbb{Z}_2 \wr \mathbb{Z}_2)$. These results deepen our understanding of the structural properties, symmetries, and geometric factors present in network.

**Theorem 1.** *[10] Let $\mathcal{N}$ be a network on $n \geq 3$ vertices and $(n-1)$ orbits. Then $O_{\mathcal{N}}(x) = x^2 + (n-2)x$ and $Aut(\mathcal{N}) \cong \mathbb{Z}_2$.*

**Theorem 2.** *[11] The graph $T$ is isomorphic to the star graph $S_n$ if and only if its edge-orbit polynomial $\bar{O}_T(x)$ is equal to $x^n - 1$.*

**Theorem 3.** *[11] Let $G$ be a graph without a pendant edge. Then $O_G(x) = \bar{O}_G(x)$ if and only if $G \cong C_n$.*

**Theorem 4.** *[12] Let $G$ be a graph of order $n$ with the orbit polynomial $O_G(x) = ax + bx^2 + cx^3$, where $a$, $b$, and $c$ are three positive integers such that $1 \leq a, b, c \leq 3$. Then the automorphism group of $G$, denoted $Aut(G)$, is a $\{2,3\}$-group, i.e., all the prime divisors of $|Aut(G)|$ are either 2 or 3.*

**Theorem 5.** *[22] Let $S$ be a set of generators of $Aut(G)$, where $1 \notin S$, and $S$ can be written as the union of disjoint subsets $S_1, S_2, \ldots, S_m$. Then, we have that $Aut(G)$ is isomorphic to the direct product $\langle S_1\rangle \times \langle S_2\rangle \times \ldots \times \langle S_m\rangle$, where each $\langle S_i\rangle$ denotes the subgroup generated by $S_i$.*

*A network $G$ that satisfies Theorem 5 is referred to as locally symmetric. More specifically, $G$ is said to be locally symmetric if its automorphism group $Aut(G)$ can be factorized into multiple geometric factors.*

*For a graph $G$ and a subset of generators $S \subseteq G$, let $supp(S)$ denote the union of supports of all elements of $S$.*

**Corollary.** *[12] Suppose $S$ is a set of generators of $Aut(G)$ without the identity 1, and $S$ can be expressed as the disjoint union $S = S_1 \cup \cdots \cup S_m$ for some $m \geq 1$. Let $t$ be the number of singleton sets in $S$. Then $O_G(x) = tx + \sum_{i=1}^{m} x^{supp(s_i)}$ and $O^\star_G(x) = 1 - tx - \sum_{i=1}^{m} x^{supp(s_i)}$.*

In Figure 6, we see a graph $K$ that exemplifies a common arrangement of symmetric subgraphs observed in many real-world networks. The automorphism group of $K$ is intricately related to the automorphism groups of the subgraphs induced by its orbits. In a prior work, the authors of [30] determined the automorphism group of $K$ to be

$$Aut(K) \cong \mathbb{Z}_2^2 \times S_3 \times S_4 \times (\mathbb{Z}_2 \wr \mathbb{Z}_2).$$

Therefore, we have $O_K(x) = 12x + 5x^2 + x^3 + 2x^4$ and $O^\star_K(x) = 1 - (11x + 6x^2 + x^3 + 2x^4)$.

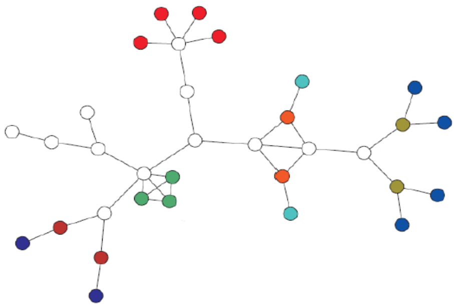


**Figure 1.** Vertices belonging to the same orbit share the same color, while singleton orbits are represented by white vertices.

## 3.2 Roots of orbit-polynomial

In this section, we begin with new results that establish the relationship between the roots of the orbit-polynomial and the properties of the graph or network. The first lemma states that the value of $\delta = \delta(G)$, is equal to 1 if and only if the graph $G$ is vertex-transitive. The next lemma states that if a graph has the trivial automorphism group, then $\delta = \frac{1}{n}$, where $n$ is the order of the graph. The third theorem asserts that this graph polynomial has a unique positive zero $\delta \leq 1$. The fourth theorem states that if a graph is not vertex-transitive, then its largest root $\delta$ is greater than or equal to $\frac{1}{n}$. This theorem provides a lower bound for the largest root of the orbit-polynomial in non-vertex-transitive graphs.

Next, we encounter a theorem that deals with graphs having two orbit sizes with corresponding multiplicities. The theorem states that the unique, positive root of the equation $O^{\star}_G(\delta) = 1-(a_{n_1} \cdot \delta^{n_1} + a_{n_2} \cdot \delta^{n_2}) = 0$ is greater than $\frac{1}{1+M}$, where $M$ is the maximum of the multiplicities $a_{n_1}$ and $a_{n_2}$. This result provides a relationship between $\delta$ and the multiplicities of the orbit sizes in the graph.

The subsequent theorem considers the case where one of the orbit sizes is fixed while the other varies. It establishes a relationship between the roots $\delta_1$ and $\delta_2$ of the equation $O^{\star}_G(\delta) = 1-(a_{n_1}\delta^{n_1} + a_{n_2}\delta^{n_2}) = 0$, when $n_1$ is fixed but $n_2$ varies. If $\delta_2 > \delta_1$, then the theorem provides an inequality relating $n_2$ and the values of $\delta_1$ and $\delta_2$. This result allows us to compare the roots of the equation for different values of $n_2$.

The following two theorems, consider the orbit polynomial and modified orbit polynomial $O_G^\star$ and their zeros. The first theorem states that for a graph on $n$ vertices, all the zeros of the modified orbit polynomial lie in the disc $C = \{z\in\mathbb{C} : |z| < \frac{1+\sqrt{8n}}{2}\}$. This result provides a geometric constraint on the location of the zeros of the modified orbit polynomial.

The second theorem states that for a network on $n$ vertices that is not vertex-transitive and has a non-identity automorphism, all zeros of the orbit polynomial lie in the interval $\left(\frac{-1}{n-2}, n-2\right]$. The subsequent theorem provides another condition for the roots of the orbit polynomial in a network. It states that if for each $i$ in the range 1 to $n$, $m \leq \sqrt[i]{a_i}$, where $a_i$ is the coefficient of $x^i$ in the orbit polynomial, then $\delta$ is in the interval $(0, \frac{1}{m}]$. The penultimate theorem asserts that for any rational number $\alpha$ in the interval $(-\infty, 0]$, there exists a network such that the orbit polynomial evaluated at $\alpha$ is 0. Furthermore, it states that the set of all roots of the orbit polynomial is dense. This result implies that the roots of the orbit polynomial can take on a wide range of values.

Finally, the last theorem considers the case where a network has an orbit of order $n - i$, where $i$ is less than or equal to half the number of vertices $n$. It states that $\delta$ is in the interval $(\frac{1}{i+1}, 1)$.

Overall, these results provide insights into the roots of the orbit-polynomial in various graph and network structures. They establish relationships between $\delta$ and graph properties such as vertex-transitivity, multiplicities of orbit sizes, and coefficients of the orbit polynomial.

**Lemma 1.** *[5] $\delta(G) = 1$ if and only if $G$ is vertex-transitive.*

**Lemma 2.** *[5] Let $G = (V, E)$ be a graph of order $n$. If $G$ has the trivial automorphism group, then $\delta(G) = \frac{1}{n}$.*

**Theorem 6.** *[5] The graph polynomial $O_G^\star(z) = 1 - O_G(z)$ has a unique positive zero $\delta < 1$.*

**Theorem 7.** *[5] Let $G = (V, E)$ be a graph and $|V| = n$ which is not vertex-transitive. Then $\delta(G) \geq \frac{1}{n}$.*

**Theorem 8.** *[6] Let $G = (V, E)$ be a graph with two orbit sizes $n_1$ and $n_2$ with corresponding multiplicities $a_{n_1}$ and $a_{n_2}$, respectively, so that $a_{n_1} \cdot n_1 + a_{n_2} \cdot n_2 = |V|$. Let $\delta$ be the unique, positive root of the equation $O^{\star}_G(\delta) = 1 - (a_{n_1} \cdot \delta^{n_1} + a_{n_2} \cdot \delta^{n_2}) = 0$. Then $\delta > \frac{1}{1+M}$, where $M := \max\{a_{n_1}, a_{n_2}\}$.*

**Theorem 9.** *[6] Let $G = (V, E)$ be a graph with two orbit sizes $n_1$ and $n_2$ with corresponding multiplicities $a_{n_1}$ and $a_{n_2}$, respectively, so that $a_{n_1} \cdot n_1 + a_{n_2} \cdot n_2 = |V|$. Let $\delta_1$ be the zero of $O^{\star}_G(\delta) = 1 - (a_{n_1}\delta^{n_1} + a_{n_2}\delta^{n_2}) = 0$, where $n_1$ and $n_2$ are fixed, but arbitrary. Assuming $n_1$ is fixed, but $n'_2$ varies, let $\delta_2$ be the root of the equation $O^{\star}_G(\delta) = 1-(a_{n_1}\delta_2^{n_1} + a_{n'_2}\delta_2^{n'_2}) = 0$.*

*If $\delta_2 > \delta_1$, then $n'_2 > \dfrac{\ln(\frac{1-a_{n_1}\delta_1^{n_1}}{a_{n'_2}})}{\ln(\delta_1)}$.*

**Theorem 10.** *[10] Suppose $G$ is a graph on $n$ vertices, then all zeros of modified orbit polynomial $O^{\star}_G$ lie in disc $C = \{z \in \mathbb{C} : |z| < \frac{1+\sqrt{8n}}{2}\}$.*

**Theorem 11.** *[10] Let $\mathcal{N}$ be a network on $n \geq 3$ vertices that is not vertex-transitive and $Aut(\mathcal{N}) \neq id$, with the orbit polynomial $O_{\mathcal{N}}(x) = \sum_{i=1}^{t} a_i x^i$. Then all zeros lie in $\left(\frac{-1}{n-2}, n-2\right]$.*

**Theorem 12.** *[10] Let $\mathcal{N}$ be a network on $n \geq 3$ vertices with the orbit polynomial $O_{\mathcal{N}}(x) = \sum_{i=1}^{t} a_i x^i$ and $O^{\star}{}_{\mathcal{N}}(x) = 1 - \sum_{i=1}^{t} a_i x^i$. If for $i \in \{1, 2, \ldots, n\}$, $m \leq \sqrt[i]{a_i}$, then $\delta \in (0, \frac{1}{m}]$.*

**Theorem 13.** *[10] For any rational number $\alpha$ in the interval $(-\infty, 0]$ there is a network $\mathcal{N}$ such that $O_{\mathcal{N}}(\alpha) = 0$. More generally, the set of all roots of $O_{\mathcal{N}}$ is dense.*

**Theorem 14.** *[10] If the network $\mathcal{N}$ has an orbit of order $n - i$ ($i \leq \frac{n}{2}$), then $\delta \in (\frac{1}{i+1}, 1)$.*

## 3.3 Graphs with three different orbit sizes

In this section, we will focus on creating graphs with predetermined orbit orders. This is possible due to the classification of 2-orbit graphs, which is discussed in the reference [10]. We will begin by exploring graphs with three orbits. The first theorem as stated in the citation [6], provides an important result regarding the positive root $\delta$ of the equation $O^*_G(\delta) = 1 - (a_{n_1} \cdot \delta^{n_1} + a_{n_2} \cdot \delta^{n_2} + a_{n_3} \cdot \delta^{n_3}) = 0$. It establishes that $\delta$ must be greater than $\frac{1}{1+M}$, where $M$ is the maximum among the multiplicities $a_{n_1}$, $a_{n_2}$, and $a_{n_3}$. This theorem provides a lower bound for $\delta$ in graphs with three orbit sizes.

The second theorem, from [6] considers the same setting but assumes fixed values for $n_2$ and $n_3$, while allowing $n_1$ to vary without bound. It states that the limiting value of the positive root $\delta$ as $n_1$ increases is the solution to the equation $-a_{n_2} \cdot \delta^{n_2} - a_{n_3} \cdot \delta^{n_3} + 1 = 0$. The third theorem introduces the concept of fixed and varying orbit sizes. The graph $G$ has three orbit sizes $n_1$, $n_2$, and $n_3$, with corresponding multiplicities $a_{n_1}$, $a_{n_2}$, and $a_{n_3}$. The theorem considers two roots, $\delta_1$ and $\delta_2$. $\delta_1$ is the root of the equation $O^\star_G(\delta) = 1 - (a_{n_1}\delta^{n_1} + a_{n_2}\delta^{n_2} + a_{n_3}\delta^{n_3}) = 0$, when $n_1$, $n_2$, and $n_3$ are fixed, but arbitrary. $\delta_2$ is the root of the equation $O^\star_G(z) = 1 - (a_{n'_1} \cdot \delta_2^{n'_1} + a_{n_2} \cdot \delta_2^{n_2} + a_{n_3} \cdot \delta_2^{n_3}) = 0$, where $n_1$ varies while $n_2$ and $n_3$ remain fixed. The theorem establishes a relationship between $\delta_1$ and $\delta_2$, stating that if $\delta_2 > \delta_1$, then $n'_1 > \frac{\ln(\frac{1-a_{n_2}\delta_1^{n_2}-a_{n_3}\delta_1^{n_3}}{a_{n'_1}})}{\ln(\delta_1)}$.

Lastly, the fourth theorem, cited from [6], focuses on a specific equation $O^\star_G(z) = 1 - (2z^n + z) = -2z^n - z + 1 = 0$. The theorem states that the unique positive root $\delta$ of this equation satisfies $\delta \geq \frac{1}{3}$.

**Theorem 15.** *[6] Consider a graph $G = (V, E)$ with three orbit sizes $n_1$, $n_2$, $n_3$, and their corresponding multiplicities $a_{n_1}$, $a_{n_2}$, $a_{n_3}$ such that $a_{n_1} \cdot n_1 + a_{n_2} \cdot n_2 + a_{n_3} \cdot n_3 = |V|$. The positive root of the equation $1 - (a_{n_1} \cdot \delta^{n_1} + a_{n_2} \cdot \delta^{n_2} + a_{n_3} \cdot \delta^{n_3}) = 0$ is denoted by $\delta$. Then, it follows that $\delta > \frac{1}{1+M}$, where $M := \max\{a_{n_1}, a_{n_2}, a_{n_3}\}$.*

**Theorem 16.** *[6] Let $G = (V, E)$ be a graph with three orbit sizes $n_1$, $n_2$, $n_3$, with corresponding multiplicities $a_{n_1}$, $a_{n_2}$, $a_{n_3}$, so that $a_{n_1} \cdot n_1 + a_{n_2} \cdot n_2 + a_{n_3} \cdot n_3 = |V|$. Let $\delta$ be the unique, positive root of the equation $O^\star_G(z) = 1-(a_{n_1} \cdot \delta^{n_1} + a_{n_2} \cdot \delta^{n_2} + a_{n_3} \cdot \delta^{n_3}) = 0$. We assume that the numbers $n_2$ and $n_3$ are fixed, but arbitrary, and $n_1$ is unbounded. The limiting value of $\delta \in (0, 1)$ is the root of the equation $-a_{n_2} \cdot \delta^{n_2} - a_{n_3} \cdot \delta^{n_3} + 1 = 0$.*

**Theorem 17.** *[6] Let $G = (V, E)$ be a graph with three orbit sizes $n_1$, $n_2$, $n_3$, and corresponding multiplicities $a_{n_1}$, $a_{n_2}$, $a_{n_3}$, such that $a_{n_1} \cdot n_1 + a_{n_2} \cdot$*

$n_2 + a_{n_3} \cdot n_3 = |V|$. *Let* $\delta_1$ *be the zero of* $O_G^{\star}(\delta) = 1 - (a_{n_1}\delta^{n_1} + a_{n_2}\delta^{n_2} + a_{n_3}\delta^{n_3}) = 0$, *assuming fixed but arbitrary values for* $n_1$, $n_2$, $n_3$. *Let* $\delta_2$ *be the root of the equation* $O_G^{\star}(z) = 1 - (a_{n_1'} \cdot \delta_2^{n_1'} + a_{n_2} \cdot \delta_2^{n_2} + a_{n_3} \cdot \delta_2^{n_3}) = 0$, *where we assume fixed values for* $n_2$, $n_3$ *but vary* $n_1$. *If* $\delta_2 > \delta_1$, *then* $n_1' > \frac{\ln\left(\frac{1 - a_{n_2}\delta_1^{n_2} - a_{n_3}\delta_1^{n_3}}{a_{n_1'}}\right)}{\ln(\delta_1)}$.

**Theorem 18.** *[6] The positive root* $\delta$ *of the equation* $O_G^{\star}(z) = 1 - (2z^n + z) = -2z^n - z + 1 = 0$ *is such that* $\delta \geq \frac{1}{3}$.

Dehmer et al. [5] propose that the measure $\delta$ can be used as a relative indicator of a graph's symmetry. If the value of $\delta(G_1)$ is greater than that of $\delta(G_2)$, it is reasonable to infer that $G_1$ exhibits more symmetry compared to $G_2$, based on the counts and sizes of their respective automorphism group orbits. By applying this symmetry measure to a set of graphs $G$, a rank order can be established: $\delta(G[1]) > \delta(G[2]) > ... > \delta(G[n])$. This rank order defines a partial ordering of the graphs.

The authors aim to demonstrate the comparative symmetry of graphs from different classes using their corresponding $\delta$ values. Their analysis affirms that the $\delta$ values accurately reflect the symmetry of the graphs. Additionally, the authors derive explicit expressions for special orbit polynomials for branched trees. The motivation behind considering these graph classes stems from their utility in various disciplines such as chemistry and bioinformatics. These structures often serve as fundamental components for understanding complex systems based on networks. Linear and branched trees, including linear and branched alkanes, play significant roles in chemistry, drug design, and related fields. Therefore, it is essential to characterize these structures using quantitative measures like $\delta$ and establish interrelations between different graph classes.

For instance, the authors examine the roots of the orbit polynomials for the trees $P_n$ and $P_n^{b_1}$, where $P_n^{b_1}$ is formed by attaching an end vertex to an "inner" vertex on the original path (see Figure 2). They present a theorem based on the comparison of these roots, which further supports their research on orbit polynomials and graph symmetry.

**Theorem 19.** *Let* $O_{P_n}(z)$ *and* $O_{P_n^{b_1}}(z)$ *be the orbit polynomials of* $P_n$ *and* $P_n^{b_1}$, *respectively, and denote the unique, positive roots of* $O_{P_n}^{\star}(z)$ *and*

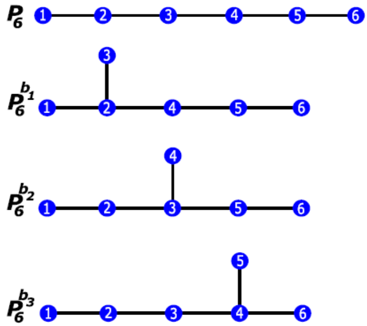
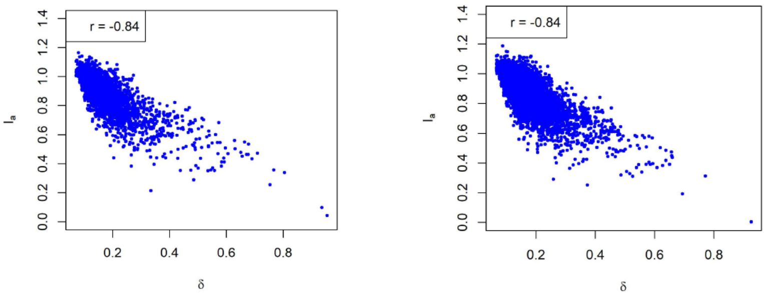



**Figure 2.** Path graph $P_6$ and branched paths $P_n^{b_1}$ , $P_n^{b_2}$, and $P_n^{b_3}$

*$O^{\star}_{P_n^{b_1}}(z)$ by $\delta(P_n)$ and $\delta(P_n^{b_1})$, respectively. The inequality $\delta(P_n) > \delta(P_n^{b_1})$ is satisfied.*

The authors examined the relationship between $\delta$ and two other symmetry measures for graphs, namely the entropy measure $I_a(G)$ and the symmetry index $S(G)$. They computed the Pearson correlation coefficient (r) between $\delta$ and these measures using exhaustively generated trees. These trees were generated using Nauty [27] and are valuable for applications in fields like chemistry, bioinformatics, and computer science due to their unique topology. It was observed that the correlation between $\delta$ and $S$ is weak. However, the correlation between $\delta$ and $I_a$ is stronger, indicating a similarity in their input, which is based on vertex orbits. The scatter plots depicted in Figures 3 and 4 further illustrate the weak correlation between $\delta$ and $S$.

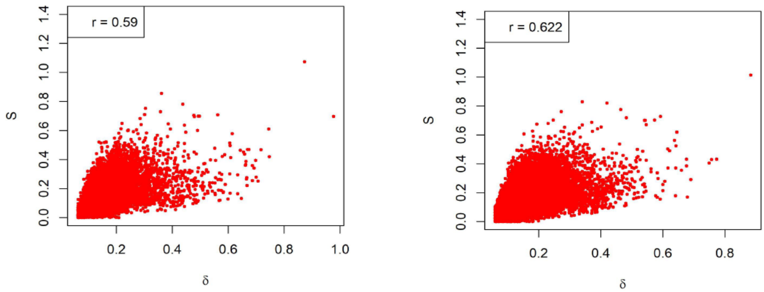
In conclusion, the analysis indicates that $\delta$, as an algebraic graph measure, possesses distinct characteristics compared to the information-theoretic measures $I_a$ and $S$. Although there are some correlations between $\delta$ and these measures, the differences in their underlying principles and reliance on vertex orbits contribute to the observed variations in correlation strength.




(a) Correlation between $\delta$ and $I_a$ based on $T_{14}$.

(b) Correlation between $\delta$ and $I_a$ based on $T_{15}$.

**Figure 3.** (a) Correlation between $\delta$ and $I_a$ based on $T_{14}$. (b) Correlation between $\delta$ and $I_a$ based on $T_{15}$.




(a) Correlation between $\delta$ and $S$ based on $T_{16}$.

(b) Correlation between $\delta$ and $S$ based on $T_{17}$.

**Figure 4.** (a) Correlation between $\delta$ and $S$ based on $T_{16}$. (b) Correlation between $\delta$ and $S$ based on $T_{17}$.

## 3.4 Achieving prescribed orbit structures in graphs: Construction and interpretation

Mowshowitz et al. [23] delve into the question of whether a given partition of a positive integer can be represented by the orbit sizes of the automorphism group of a graph. Through their work, they provide a compelling proof that demonstrates the existence of connected, undirected graphs with predetermined orbit structures within their automorphism groups. The authors accomplish this by explicitly constructing the graphs in question, ensuring that the component graphs have the minimum number of edges possible. Furthermore, they introduced a specialized class of trees that possess prescribed orbit structures. The methods developed in this research offer a valuable tool for generating graphs with a well-defined degree of symmetry.

**Theorem 20.** *[23] Let $n$ be a positive integer such that $n = \sum_{i=1}^{t} i \cdot k_i$, for some positive integer $t$, where $k_i$ is the number of values equal to $i$ in the sum. If $k_1 \leq 1$ or $k_1 \geq 6$, then there exists a graph $G$ whose automorphism group $Aut(G)$ has $t$ orbits of sizes $k_1, k_2, ..., k_t$, respectively.*

**Theorem 21.** *[23] Let $n$, $k_i$, and $t$ be as given in the hypotheses of Theorem 20, with $k_i \geq 2$ $(2 \leq i \leq t)$ and $k_i \leq k_j$ for $i \leq j$. There exists a tree with $n$ vertices whose automorphism group has $k_i$ orbits of size $i$, $2 \leq i \leq t$, and $k_1 = \sum_{i=2}^{t} k_i + \binom{k_i}{2}$.*

# 4 Application in real-world networks

In their study, Ghorbani et al. [10] examine several set of real-world networks with distinct topologies. They aim to explore the relationship between the symmetry measure $\delta$ and the orbit entropy $I_a$, as well as their correlation with the topological indices of the networks. The results reveal a significant correlation between $\delta$ and $I_a$ indicating that changes in symmetry are accompanied by variations in orbit entropy. However, no significant correlation is observed between $\delta$ and the symmetry index $S(G)$.

To further analyze the networks, various topological indices including the first Zagreb index, second Zagreb index, spectral radius, Randic index, Laplacian Estrada index, Laplacian energy, Harary index, Estrada index, energy, Balaban ID, and atom-bond connectivity, were calculated. Among these indices, the results highlight that Laplacian energy exhibits the strongest correlation with the symmetry measure $\delta$.

Overall, this study sheds light on the relationship between symmetry, orbit entropy, and various topological indices in real-world networks, providing valuable insights into the structural characteristics of these networks.

Dehmer et al. [6] explored the practical application of the symmetry measure $\delta$ by calculating it for three molecular structures. The purpose of this calculation is to demonstrate the measure's effectiveness in capturing symmetry. The authors specifically focused on hydrocarbons, which are fundamental components of mineral oils and various other products. These hydrocarbons are represented by chemical formulae of the form $C_nH_m$. The authors consider three sets of graphs for their analysis. The first set comprises isomers derived from $C_{14}H_{28}$, the second set consists of isomers derived from $C_{14}H_{26}$, and the third set includes isomers derived from $C_{14}H_{26}$ with a restriction that the structures must have two rings with a minimum size 5. The different topologies of connected carbon atoms define the set of isomers, and the authors provide examples of isomeric structures with different degrees of symmetry (see Figure 5). To demonstrate the effectiveness of the $\delta$ measure in capturing symmetry, the authors calculate $\delta$ values for three molecular structures. The calculated $\delta$ values indicate the degree of symmetry for each structure, with higher values indicating greater symmetry. The authors state that higher $\delta$ values correspond to greater symmetry, with the maximum value of $\delta$ being 1, achieved in vertex transitive graphs. In Figure 6, the histograms of the frequencies of $\delta$ values for each set are provided, showing similarities in the distributions with high frequencies at low symmetry.

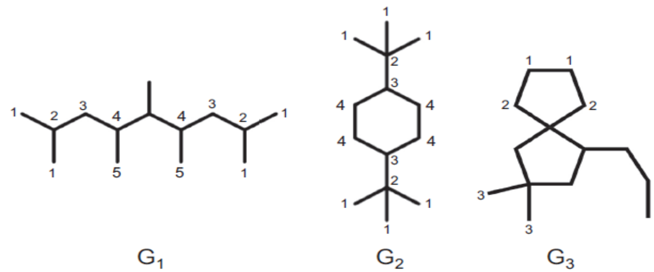



**Figure 5.** $G_1$: An isomer of the set $C_{14}H_{30}$. $\delta(G_1) = 0.307026$. $G_2$: An isomer of the set $C_{14}H_{28}$ with $\delta(G_2) = 0.626615$. $G_3$: An isomer of the set $C_{14}H_{26}$ with $\delta(G_3) = 0.119633$. The vertices are labeled by orbit numbers, where a given vertex belongs to orbit 1, 2, 3, 4, or 5. If a vertex is not labeled by a number, it represents a singleton orbit.

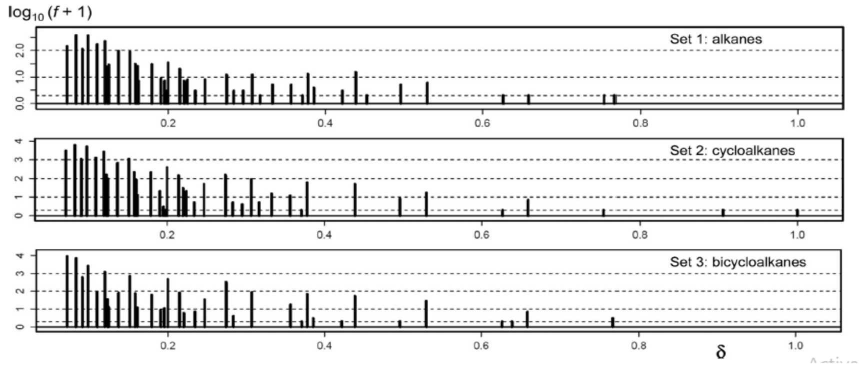



**Figure 6.** The distribution of the $\delta$-values for the three sets containing chemical structures can be visualized through a plot of frequency, $f$, as $\log_{10}(f+1)$.

The authors discuss the minimum and maximum values of $\delta$ for graphs with a given number of vertices ($C$-atoms). The minimum value of $\delta$ corresponds to asymmetric graphs, where each atom is in a separate orbit. The maximum value of $\delta$ is obtained when all atoms are in a singleton orbit, indicating maximum symmetry. Furthermore, the authors mentioned the use of automorphism groups of graphs to obtain orbit data and calculate the symmetry measure $\delta$. However, the results show that in all three sets, the numerical relationship between $\delta$ and the size of the automorphism group $|Aut(G)|$ is relatively weak. The Pearson correlation coefficients for the three sets are 0.33, 0.45, and 0.50, respectively. This suggests that there is not a strong linear correlation between $\delta$ and the size of the automorphism group in these cases. Overall, this analysis [5] explores the symmetry of chemical structures using graph representations and the $\delta$ measure. It turned out, that $\delta$ is a suitable symmetry measures as it gives meaningful values.

# 5 Summary and conclusion

In this paper, we surveyed existing results on the so-called orbit polynomial. It was introduced by Dehmer et al. [5] and brought many valuable results when exploring the symmetry of graphs. In the course of the survey, we reviewed many results where the orbit polynomial-approach got applied. In the fowllowing, we briefly sketch an idea how to generalize this approach.

If $O_G(x)$ is the orbit polynomial of $G$, then we used the equation $O_G^\star(x) = 1 - O_G(x) = 0$ to infer the unique root $\delta$ that lies between zero and one. We note that this idea can be easily generalized and used in other graph domains. So, consider the graph polynomial

$$P_G(z) = a_n z^n + \cdots + a_1 z + a_0,$$

where $a_i$ capture structural information of the graph (e.g., distances between vertices, degrees, orbit sizes etc.). If $a_0 \neq 0$, then we generalize the above stated idea bu considering $P_G^\star(z) := 1 - z \cdot P_G(z)$ to obtain the unique positive zero between $(0, 1]$. If $a_0 = 0$, then we have the case as illustrated in the survey for the orbit polynomial. Besides considering the unique and positive zero of $P_G^\star(z) := 1 - z \cdot P_G(z) = 0$ and $P_G^\star(z) := 1 - P_G(z) = 0$, we could also investigate all zeros of a graph polynomial $P_G(z)$ and $P_G^\star(z)$. This would lead to the investigation of all zeros of

$$P_G(z) = a_n z^n + \cdots + a_1 z + a_0 = 0,$$

or

$$P_G^\star(z) = 1 - (a_n z^n + \cdots + a_1 z) = 0,$$

or

$$P_G^\star(z) = 1 - z(a_n z^n + \cdots + a_1 z + a_0) = 0.$$

This would enable us to establish a direct connection to the theory of eigenvalues.

# References

[1] K. Balasubramanian, On graph theoretical polynomials in chemistry, in: N. Trinastić, (Ed.), *Mathematical and Computational Concepts in Chemistry*, Ellis Horwood Ltd., New York, 1986, pp. 20–33.

[2] K. Balasubramanian, S. C. Basak, Characterization of isospectral graphs using graph invariants and derived orthogonal parameters, *J. Chem. Inf. Comput. Sci.* **38** (1998) 367–373.

[3] K. Balasubramanian, R. Ramaraj, Computer generation of king and color polynomials of graphs and lattices and their applications to statistical mechanics, *J. Comput. Chem.* **6** (1985) 447–454.

[4] D. Cvetković, M. Doob, H. Sachs, *Spectra of Graphs Theory and Applications*, Academic Press, Heidelberg, 1995.

[5] M. Dehmer, Z. Chen, F. Emmert-Streib, A. Mowshowitz, K. Varmuza, H. Jodlbauer, Y. Shih, S. Tripathi, J. Tao, The orbit-polynomial: A novel measure of symmetry in networks, *IEEE Access* **8** (2020) 36100–36112.

[6] M. Dehmer, F. Emmert-Streib, A. Mowshowitz, A. Ilić, Z. Chen, G. Yu, L. Feng, M. Ghorbani, K. Varmuza, J. Tao, Relations and bounds for the zeros of graph polynomials using vertex orbits, *Appl. Math. Comput.* **380** (2020) #125239.

[7] E. J. Farrell, An introduction to matching polynomials, *J. Comb. Theory* **27** (1979) 75–86.

[8] E. J. Farrell, C. M. De Matas, On star polynomials of complements of graphs, *Ark. Mat.* **26** (1988) 185–190.

[9] E. J. Farrell, C. M. De Matas, Star polynomials of some families of graphs with small cyclomatic numbers, *Util. Math.* **58** (2000) 33–45.

[10] M. Ghorbani, R. Alidehi-Ravandi, M. Dehmer, F. Emmert-Streib, A study of roots of a certain class of counting polynomials, *Mathematics* **11** (2023) #2876.

[11] M. Ghorbani, M. Dehmer, F. Emmert-Streib, On the degeneracy of the orbit polynomial and related graph polynomials, *Symmetry* **12** (2020) #1643.

[12] M. Ghorbani, M. Jalali-Rad, M. Dehmer, Orbit polynomial of graphs versus polynomial with integer coefficients, *Symmetry* **13** (2021) #710.

[13] I. Gutman, Some analytical properties of the independence and matching polynomials, *MATCH Commun. Math. Comput. Chem.* **28** (1992) 139–150.

[14] I. Gutman, D. Bonchev, D. H. Rouvray, Polynomials in graph theory, in: D. Bonchev, D. H. Rouvray (Eds.), *Chemical Graph Theory – Introduction and Fundamentals*, Abacus Press, New York, 1991, pp. 133–176.

[15] I. Gutman, A survey on the matching polynomial, in: Y. Shi, M. Dehmer, X. Li, I. Gutman (Eds.), *Graph Polynomials*, CRC Press, Boca Raton, 2016, pp. 77–99.

[16] I. Gutman, B. Furtula, V. Katanić, Randić index and information, *AKCE Int. J. Graphs Comb.* **15** (2018) 307–312.

[17] I. Gutman, F. Harary, Generalizations of the matching polynomial, *Util. Math.* **24** (1983) 97–106.

[18] I. Gutman, H. Hosoya, Molecular graphs with equal $Z$-counting and independence polynomials, *Z. Naturforsch.* **45a** (1990) 645–648.

[19] H. Hosoya, Clar's aromatic sextet and sextet polynomial, *Top. Curr. Chem.* **153** (1990) 255–272.

[20] H. Hosoya, On some counting polynomials in chemistry. Applications of graphs in chemistry and physics, *Discr. Appl. Math.* **19** (1988) 239–257.

[21] H. Hosoya, Topological index. A newly proposed quantity characterizing the topological nature of structural isomers of saturated hydrocarbons, *Bull. Chem. Soc. Jpn.* **44** (1971) 2332–2339.

[22] B. D. MacArthur, R.J. Sánchez-García, J. W. Anderson, Symmetry in complex networks, *Discr. Appl. Math.* **156** (2008) 3525–3531.

[23] A. Mowshowitz, M. Dehmer, F. Emmert-Streib, A note on graphs with prescribed orbit structure, *Entropy* **21** (2019) #1118.

[24] A. Motoyama, H. Hosoya, King and domino polynomials for polyomino graphs, *J. Math. Phys.* **18** (1977) 1485–1490.

[25] T. Hahn, H. Wondratschek, *Symmetry of Crystals, Introduction to International Tables for Crystallography*, Vol. A, Heron Press, Sofia, 1994.

[26] M. Ladd, *Symmetry and Group Theory In Chemistry*, Harwood Publishers, London, 2000.

[27] B. D. McKay, A. Piperno, Practical graph isomorphism II, *J. Symb. Comput.* **60** (2014) 94–112

[28] F. G. Montoya, R. Banos, A. Alcayde, F. Manzano-Agugliaro, Symmetry in engineering sciences, *Symmetry* **11** (2019) #797.

[29] D. J. Gross, The role of symmetry in fundamental physics, *Proc. Natl. Acad. Sci.* **93** (1996) #14256.

[30] S. K. Parui, D. Dutta Majumder, Symmetry analysis by computer, *Pattern Recogn.* **16** (1983) 63–67.