mathematics

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A Study of Roots of a Certain Class of Counting Polynomials

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Abstract: In this article, we introduce a new counting polynomial, namely the orbit polynomial. It is well-known that this polynomial has a unique positive zero δ in the interval $[0,1]$. The aim of this paper is to study the specific properties of this polynomial and then determine the location of this root for several classes of complex networks to compare with other graphical measures. Additionally, we compare the unique positive zero measure with several well-known centrality graph measures.

Keywords: orbit polynomial; complex networks; automorphism group; entropy

MSC: 05C25; 05C31; 94A17

Citation: Ghorbani, M.; Ravandi-Alidehi, R.; Dehmer, M.; Emmert-Streib, F. A Study of Roots of a Certain Class of Counting Polynomials. *Mathematics* **2023**, *11*, 2876. https://doi.org/10.3390/math11132876

Academic Editor: Andrea Scozzari

Received: 7 May 2023
Revised: 12 June 2023
Accepted: 20 June 2023
Published: 27 June 2023

1. Introduction

The orbit polynomial of a graph is a polynomial that encodes information about the orbits of its automorphism group. Its roots and their properties have become an important tool for studying the symmetry structure and other structural features of networks in many different fields, including graph theory, physics, chemistry, and computer science.

On the other hand, the unique positive root of the orbit polynomial, denoted δ, has gained particular attention due to its ability to serve as a structural descriptor for networks. δ has been shown to provide insight into the symmetry structure of a graph, with its value being closely related to the size and complexity of its automorphism group. This line of research has given rise to a range of applications of δ in network analysis, including the classification and comparison of different types of networks.

Overall, the study of the roots of the orbit polynomial of networks has opened up new avenues for research into the structural properties of networks, with many potential applications in various fields. Ongoing efforts are addressing open questions related to the computation, properties, and applications of the orbit polynomial and its roots, with the aim of furthering our understanding of the structure of networks and their applications in many different areas of science.

In computing the orbit polynomial of a network, not only the group Γ is important but also the orbit-set $\mathcal{X}$ has a vital role in computing the orbit polynomial. In other words, for two isomorphic but not permutationally isomorphic permutation groups Γ_1 and Γ_2, we may obtain distinct orbit polynomials. This means that the cycle type of all permutations or at least the cycle type of the generators of the automorphism group has a significant role in the structure of orbit polynomial.

We proceed as follows: Section 2 outlines the concepts and definitions that will be used in this paper. In Section 3, we compute the several bounds for the roots of M-orbit polynomial. Finally, in Section 4, we compute some topological indices for certain networks such as *Human B Cell*, *BioGRID Drosophila*, *US Airports*, and *Email* with QuACN-package [1].

2. Preliminaries

In this paper, we utilize standard notation from graph theory, as presented in [2]. The vertex set and edge set of network $\mathcal{N}$ are denoted by $V(\mathcal{N})$ and $E(\mathcal{N})$, respectively. All networks are simple, connected, and finite.

Given network $\mathcal{N}$ and an arbitrary vertex $v \in V(\mathcal{N})$, we define the vertex orbit (or orbit of v) as the set of all vertices $\alpha(v)$, where α is an automorphism of $\mathcal{N}$.

Recently, the concept of orbit polynomial [3] for a connected network $\mathcal{N}$ was defined as follows:

$$\mathbb{O}_{\mathcal{N}}(x) = \sum_{i=1}^{t} x^{|\mathbb{O}_i|},$$

where $\mathbb{O}_1, \mathbb{O}_2, \ldots, \mathbb{O}_t$ are all vertex orbits of $\mathcal{N}$ and the cardinallity of an orbit is denoted by $|\mathbb{O}_i|$. Moreover, the modified version of this polynomial or M-orbit polynomial is defined as

$$\mathbb{O}^{\star}_{\mathcal{N}}(x) = 1 - \sum_{i=1}^{t} x^{|\mathbb{O}_i|}. \tag{1}$$

The definition of this polynomial is based on two concepts: the automorphism group and the vertex orbits. It is well-known that the orbit polynomial has a unique positive zero δ in the interval $[0, 1]$, see [3].

Ghorbani et al. in [4] generalized the concept of orbit polynomial as follows: consider the action of permutation group Γ acting on the set X. Then, the generalized orbit polynomial is $\mathbb{O}_{\Gamma}(x) = \sum_{i=1}^{t} c_i x^{|\mathbb{O}_i|}$, where $\mathbb{O}_1, \ldots, \mathbb{O}_t$ are all orbits of Γ. It is clear that for a graph $\mathcal{N}$ with automorphism group $Aut(\mathcal{N})$, $\mathbb{O}_{\Gamma}$ equals the ordinary orbit polynomial.

In our research, we utilized the *i*-graph package [5] to assist in computing the automorphism group and orbits of the networks under consideration.

3. Location of Roots

In [6], several bounds for the positive root δ are given and some properties of the orbit polynomial are investigated. In this section, we obtain several results concerning the location of zeros of the modified orbit polynomial. The following proposition sharpens previous results along with some of the other known results which were based on Walsh's classical theorem. Moreover, an R-code is developed to construct polynomials and compare the bounds obtained by our result with these known results.

Proposition 1. *Let $f(z) = \sum_{k=0}^{n} a_k z^k$, $(a_k \neq 0)$ be a non-constant polynomial with complex coefficients. Then all its zeros lie in disc $C = \{z \in \mathbb{C} : |z| \leq r\}$, where*

(i) $r < 1 + \max_{0 \leq k \leq n-1}\{|a_k|\}$, [7]

(ii) *(Walsh)* $r = \sum_{k=0}^{n-1} |a_k|^{1/(n-k)}$, [8]

(iii) *(Carmichael et al.)* $r = \sqrt{1 + \sum_{k=0}^{n-1} |a_k|^2}$ [9] .

We recall that a graph is vertex-transitive if it only has one vertex orbit. It is not difficult to see that, if G is a vertex-transitive graph, then $\mathbb{O}_G(x) = x^n$, $\mathbb{O}^{\star}_G(x) = 1 - x^n$, and thus its positive real root is one. Furthermore, if $\mathbb{A}_G \cong id$ (namely, G is asymmetric graph with identity automorphism group), then $\mathbb{O}_G(x) = nx$, $\mathbb{O}^{\star}_G(x) = 1 - nx$ and its positive real root is $\frac{1}{n}$. This yields that for a given graph G on n vertices, which is neither vertex-transitive nor an identity graph, then positive root $\delta \in (\frac{1}{n}, 1)$.

In the case that G is not vertex-transitive and $\mathbb{A}_G \neq id$, then clearly we have $0 \leq a_i \leq n - 2$ and according to Proposition 1(i) , it can be verified that $r < n - 1$ and $0 < |z| < n - 1$. By Proposition 1(ii), we obtain

$$r = {a_0}^{1/n} + a_1^{1/n-1} + \ldots + a_{n-2}^{1/2} + a_{n-1}. \tag{2}$$

For $i > [n/2]$ ([] denotes to the floor function) , it is clear that $a_i \in \{0,1\}$ and only one of a_i's is 1. On the other hand, if the order of orbits is smaller than $[n/2]$, the number of terms in Equation (2) will be increased and thus the value of r will be too.The maximum number of terms holds if all a_i's are one. Since $\sum_{i=1}^{n} ia_i = n$, a graph in which $n = 1 + 2 + 3 + \cdots + m$ (for some integer m), has the largest value of r. Hence, $m = \frac{-1+\sqrt{8n}}{2}$ and so $r \leq 1 + m = \frac{1+\sqrt{8n}}{2}$, or equivalently $|z| < \frac{1+\sqrt{8n}}{2}$.

If the number of terms in Equation (2) decreases, the value of r will decrease and if the orders of the orbits of the graph are equal, then Equation (2) will be a monomial. It is not difficult to see that by Proposition 1(*ii*), the minimum value of r is $r \geq 1 + 2^{2/n} > 2$, in which $\mathbb{O}^{\star}_{G}(x) = 1 - 2x^{n/2}$. By Proposition 1(*iii*), we have

$$r = \sqrt{1 + \sum_{k=0}^{n-1} |a_k|^2} = \sqrt{1 + (1^2 + {a_1}^2 + {a_2}^2 + \ldots + {a_{n-1}}^2)}.$$

Knowing that the graph is not vertex-transitive and $\mathbb{A}_G \neq id$, it can be inferred that $2 \leq \sum a_i \leq n - 1$, and thus

$$\sum {a_i}^2 < (\sum a_i)^2 \leq (n-1)^2,$$

or equivalently,

$$r < \sqrt{2 + (n-1)^2} = (n-1)\sqrt{1 + \frac{2}{(n-1)^2}}.$$

Thus, if $n \geq 3$, we may conclude that $r < (n-1)\sqrt{\frac{3}{2}}$. The lower bound for r using Proposition 1(*iii*) is (G is not vertex-transitive and $\mathbb{A}_G \ncong id$)

$$r \geq \sqrt{1 + (1^2 + 1^2 + 1^2)} = 2 \ \ (a_{n-1}, a_1 = 1).$$

Hence, we proved the following theorem.

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

Corollary 1. *For the star graph* S_n *with n vertices,* $\mathbb{O}_{S_n}(x) = x + x^{n-1}$ *and all the zeros of* $\mathbb{O}^{\star}_{S_n}(x) = 1 - (x + x^{n-1})$ *lie in* $[-2, 2]$.

Theorem 2 ([9])**.** *Let*

$$f(z) = a_n z^n + a_{n-1} z^{n-1} + \ldots + a_0, \ a_n a_{n-1} \neq 0,$$

be a complex polynomial. All zeros of $f(z)$ *lie in*

$$|z| \leq \frac{1+\phi}{2} + \frac{\sqrt{(\phi-1)^2 + 4M_2}}{2},$$

where

$$\phi := \left|\frac{a_{n-1}}{a_n}\right|,$$

and

$$M_2 := \max_{0 \leq j \leq n-2} \left|\frac{a_j}{a_n}\right|.$$

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

Proof. We know that $a_i \leq n-2$; therefore Theorem 2 implies that

$$Max\phi = \frac{n-2}{1} = n-2.$$

Hence, the orbit polynomial is of form $x^2 + (n-2)x$ and so $M_2 = 0$. Consequently,

$$z \leq \frac{1+(n-2)}{2} + \frac{\sqrt{(n-3)^2}}{2} = n-2.$$

Also

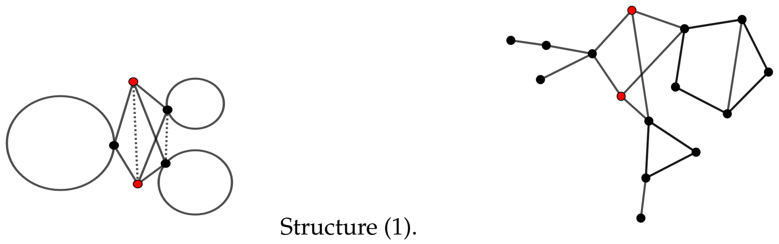
$$Min\phi = \frac{1}{n-2}.$$

Thus, the orbit polynomial is $(n-2)x^2 + x$. Since $M_2 = 0$ and $\sum_{i=1}^{t} ia_i = n$, we conclude that $n = 3$. This means that if $n > 3$, there is no graph with $Min\phi = \frac{1}{n-2}$. ☐

Theorem 4. *Let $\mathcal{N}$ be a network on $n \geq 3$ vertices and $(n-1)$ orbits. Then $\mathbb{O}_{\mathcal{N}}(x) = x^2 + (n-2)x$ and $\mathbb{A}_{\mathcal{N}} \cong \mathbb{Z}_2$.*

Proof. Since $\mathcal{N}$ has $(n-1)$ orbits, one can easily conclude that there are $(n-2)$ singleton orbits and an orbit of order 2. This completes the proof. ☐

Example 1. *We utilized the Sage software [10] to analyze all networks up to the order of 10 and made an observation about the structure of graphs with orbit polynomial $O_{\mathcal{N}}(x) = x^2 + (n-2)x$. Our finding revealed that the structure of such graphs falls under one of the categories illustrated in Figure 1.*



Structure (1). An example of structure (1).

Structure (2). An example of structure (2).

Structure (3). An example of structure (3).

Figure 1. *Cont.*

Structure (4). An example of structure (4).

Structure (5). An example of structure (5).

Figure 1. All structures of graphs with $O_{\mathcal{N}}(x) = x^2 + (n-2)x$.

The Location of Positive Real Root δ

In the last section, we showed that $\delta \in [\frac{1}{n}, 1]$. In addition, in [11], it was shown that as δ increases toward one, the graph becomes more symmetric, and as δ tends to zero, the graph will be less symmetric, especially for sufficiently large values of n. After our previous discussions, the objective of this section is to devise a framework that can effectively examine the conduct of the positive real root of the modified orbit polynomial.

Theorem 5. *Let $\mathcal{N}$ be a network on $n \geq 3$ vertices with the orbit polynomial $\mathbb{O}_{\mathcal{N}}(x) = \sum_{i=1}^{t} a_i x^i$ and $\mathbb{O}^{\star}{}_{\mathcal{N}}(x) = 1 - \sum_{i=1}^{t} a_i x^i$. If for $i \in \{1, 2, \ldots, n\}$, $m \leq \sqrt[i]{a_i}$, then $\delta \in (0, \frac{1}{m}]$.*

Proof. $\mathbb{O}^{\star}_{\mathcal{N}}(\frac{1}{m}) = 1 - (\frac{1}{m}a_1 + \frac{1}{m^2}a_2 + \ldots + \frac{1}{m^i}a_i + \ldots + \frac{1}{m^t}a_t) \leq 0$, considering that $\mathbb{O}^{\star}_{\mathcal{N}}(0) > 0$ and $\mathbb{O}^{\star}_{\mathcal{N}}(1) < 0$, it can be concluded $\delta \in (0, \frac{1}{m}]$. $\square$

Example 2. *Let $\mathcal{N}$ be a network with the orbit polynomial $\mathbb{O}_{\mathcal{N}}(x) = 4x + 7x^2 + 25x^3$ and $\mathbb{O}^{\star}{}_{\mathcal{N}}(x) = 1 - (4x + 7x^2 + 25x^3)$. Since $a_1 = 4$, we may conclude that $m \leq 4$ and $a_2 = 7$ gives $m^2 \leq 7$. Furthermore, $a_3 = 25$ yields $m^3 \leq 25$ and thus $\max(m) = 4$ and $\delta \in (0, \frac{1}{4}]$.*

Corollary 2. *The value $\delta = \frac{1}{2}$ holds for a network with orbit polynomial $\mathbb{O}_{\mathcal{N}}(x) = 2^i x^i$ and if the network $\mathcal{N}$ has k singleton orbits, then the positive real root $\mathbb{O}^{\star}{}_{\mathcal{N}}(x)$ lies in $(0, \frac{1}{k}]$.*

Theorem 6. *For any rational number α in the interval $(-\infty, 0]$ there is a network $\mathcal{N}$ such that $\mathbb{O}_{\mathcal{N}}(\alpha) = 0$. More generally, the set of all roots of $\mathbb{O}_{\mathcal{N}}$ is dense.*

Proof. Let $a, b \in \mathbb{N}$. There is a network of order $n = a + 2b$ such that $\mathbb{O}_{\mathcal{N}}(x) = ax + bx^2$. An example of such networks is shown in Figure 2. It is enough to have a network with a vertices and putting two pendant vertices in the position of the b vertices, such that no pair of vertices on the path P_b can be permuted to each other. $\square$

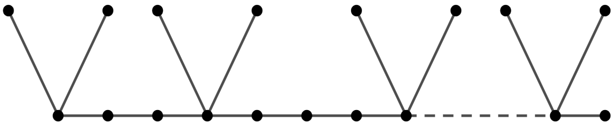


Figure 2. An example of a graph with orbit polynomial $\mathbb{O}_{\mathbb{N}}(x) = ax + bx^2$.

Theorem 7. *If the network $\mathcal{N}$ has an orbit of order $n - i$ ($i \leq \frac{n}{2}$), then $\delta \in (\frac{1}{i+1}, 1)$.*

Proof. It is clear that $a_{n-i} = 1$ and i vertices lie in orbits by order smaller than $\frac{n}{2}$. Thus, the orbit polynomial as follows: $\mathbb{O}_{\mathcal{N}}(x) = a_1x^1 + a_2x^2 + \ldots + a_kx^k + x^{n-i}(k < \frac{n}{2})$. The maximum value of $\mathbb{O}_{\mathcal{N}}(\delta)$ holds if $\mathbb{O}_{\mathcal{N}}(x) = ix(a_1 = i)$ and $\mathbb{O}^{\star}_{\mathcal{N}}(\frac{1}{i+1}) = i(\frac{1}{i+1}) < 1$. This means that $\delta \in (\frac{1}{i+1}, 1)$.

The maximum value of $\mathbb{O}_{\mathcal{N}}(\delta)$ holds if $\mathbb{O}_{\mathcal{N}}(x) = ix + x^{n-i}(a_1 = i)$ and $\mathbb{O}^{\star}_{\mathcal{N}}(\frac{1}{i+1}) = 1 - (i(\frac{1}{i+1}) + (\frac{1}{i+1})^{n-i}) > 0$. This means that $\delta \in (\frac{1}{i+1}, 1)$. □

Theorem 8. *Suppose the tree T has an orbit of order* 2 $(|\mathbb{O}_i| = 2)$ *and the other orbits are singleton, then* $\langle \mathbb{O}_i \rangle \cong P_3$.

Proof. If $\mathbb{O}_i = \{y, z\}$, it is clear that there is an automorphism such as φ so that $\varphi(y) = z$. Now, if y and z lie in different branches of T such as B_1 and B_2, then it follows from $\varphi(y) = z$ that $\varphi(B_1) = B_2$, a contradiction. Therefore y and z are in the same branch such as B. Let us assume that the root of the branch B is x,and the paths from y and z to x are denoted by p_1 and p_2, respectively. So $\varphi(p_1) = p_2$ and if t is a vertex on p_1, then there is a vertex such as t' on p_2 which $\varphi(t) = t'$ that is contradiction. Hence, $d(x, y) = d(x, z) = 1$ and the issue is confirmed. □

Corollary 3. *Let T be a tree on* $n \geq 3$ *vertices and* $\mathbb{O}_{\mathcal{T}}(x) = x^2 + (n-2)x$, *then*

$$\delta = \frac{2}{\sqrt{(n-2)^2 + 4} + (n-2)}.$$

Proof. Suppose $\mathbb{O}^{\star}_{T}(x) = 1 - (x^2 + (n-2)x)$, then clearly the roots are

$$x_{1,2} = \frac{-(n-2) \pm \sqrt{(n-2)^2 + 4}}{2}$$

and thus

$$\delta = \frac{2}{\sqrt{(n-2)^2 + 4} + (n-2)}.$$

This completes the proof. □

Corollary 4. *Let T be a tree on n vertices:*

(1) If $\mathbb{A}_T \cong id$, *then* $\delta = \frac{1}{n}$.

(2) If $\mathbb{A}_T \neq id$, *then* $\delta \in [\alpha, 1]$ *so that*

$$\alpha = \frac{\sqrt{(n-2)^2 + 4} - (n-2)}{2}.$$

4. The Role of δ in the Study of Real Network Structures

Complex networks have been extensively studied in various fields in recent years. The concept of entropies has been used to characterize and quantify the structure of networks and has been investigated in many studies [12–19]. To define graph entropies, we adopt Dehmer's definition [20], which relies on probability vector $p = (p_1, \ldots, p_n)$, satisfies two conditions: $0 \leq p_i \leq 1$ and $\sum_{i=1}^{n} p_i = 1$. Shannon's entropy is then defined as

$$I(p) = \sum_{i=1}^{n} p_i log(p_i).$$

Mowshowitz and Dehmer [21–23] introduced the symmetry index $S(G)$, which is defined as

$$\begin{aligned} S(G) &= (logn - I_a(G)) + log|\mathbb{A}_G| \\ &= \frac{1}{n}(\sum_{i=1}^{t} |Oi|log|Oi|) + log|\mathbb{A}_G|. \end{aligned}$$

If $I(G)$ and $I(H)$ are two graph invariants of graphs G and H, respectively, the graph distance measure between $I(G)$ and $I(H)$ is defined as $d_I(G, H) = 1 - e^{-(\frac{I(G)-I(H)}{\sigma})^2}$, according to [23]. The values of orbit entropy I_a, size of the automorphism group, symmetric index $S(G)$, unique positive real root δ, distance measure between δ and I_a, and distance measure between δ and $S(G)$ of biological and technological networks are reported in Table 1.

Table 1. Some graph measures of biological and technological networks [24].

	n	$\lvert\mathbb{A}\rvert$	δ	I_a	S	$d(\delta, I_a)$	$d(\delta, S)$
Human B CellGenetic	5930	5.94×10^{13}	1710×10^{-7}	3.77	13.8	14.20	189.83
Caenorhabditiselegans Genetic	2060	6.99×10^{161}	6258×10^{-7}	3.20	161.96	10.22	26.23×10^{3}
BioGRID Human	7013	1.26×10^{485}	1764×10^{-7}	3.73	485.2	13.93	23.54×10^{4}
BioGRID Saccharomyccscerevisiae	5295	6.86×10^{64}	1958×10^{-7}	3.70	64.86	13.71	4206.4
BioGRID Drosophila	7371	3.07×10^{493}	1690×10^{-7}	3.76	493.6	14.10	24.36×10^{4}
BioGRID Mus musculus	209	5.35×10^{125}	$221{,}440 \times 10^{-7}$	1.46	126.59	2.06	16.02×10^{3}
Yeast Protein Interactions	1458	1.07×10^{254}	$11{,}599 \times 10^{-7}$	2.88	254.30	8.31	64.67×10^{3}
c. elegans metabolic	453	1.93×10^{10}	$25{,}702 \times 10^{-7}$	2.60	10.33	6.78	106.79
Internet	22,332	$1.28 \times 10^{11{,}298}$	1035×10^{-7}	3.67	11.3×10^{3}	13.44	12.77×10^{7}
US Power Grid	4941	5.18×10^{152}	2380×10^{-7}	3.63	152.77	13.20	23.34×10^{3}
US Airports	332	2.59×10^{24}	$40{,}472 \times 10^{-7}$	2.39	24.54	5.71	602.07
www California searchsubnet	5925	1.24×10^{1298}	2820×10^{-7}	3.45	1298.4	11.93	16.86×10^{5}
www EPA.gov subnet	4253	1.28×10^{2321}	4992×10^{-7}	2.91	2321.8	8.47	53.91×10^{5}
www Political Blogs	1222	2.40×10^{35}	8741×10^{-7}	3.04	35.43	9.25	1254.9
Email	1133	1.53×10^{9}	9216×10^{-7}	3.04	9.20	9.23	84.62
Media ownership	4475	3.36×10^{4818}	$13{,}278 \times 10^{-7}$	2.16	4820.01	4.68	23.23×10^{6}
Geometry Co-authorship	3621	1.90×10^{320}	4419×10^{-7}	3.38	320.45	11.45	10.27×10^{4}
Erdös Collaboration	6927	3.46×10^{4222}	5491×10^{-7}	2.956	4223.4	8.73	17.84×10^{6}
PhD network	1025	2.98×10^{292}	$25{,}245 \times 10^{-7}$	2.55	292.93	6.49	85.81×10^{3}

Table 2 shows that the correlation values of δ and I_a in biological and technological networks are very close. However, it appears that there may be differences in the effective variables that contribute to the structure of social networks compared to other types of networks. This suggests that further research should be conducted to investigate these differences.

Table 2. The correlation values.

Biological Networks	**Technological Networks**	**Social Networks**
$\left(\begin{array}{c\|ccc} & \delta & I_a & S \\ \hline \delta & 1 & -0.88 & -0.20 \\ I_a & -0.88 & 1 & 0.33 \\ S & -0.20 & 0.33 & 1 \end{array}\right)$	$\left(\begin{array}{c\|ccc} & \delta & I_a & S \\ \hline \delta & 1 & -0.86 & -0.37 \\ I_a & -0.86 & 1 & 0.48 \\ S & -0.37 & 0.48 & 1 \end{array}\right)$	$\left(\begin{array}{c\|ccc} & \delta & I_a & S \\ \hline \delta & 1 & -0.64 & -0.19 \\ I_a & -0.64 & 1 & -0.55 \\ S & -0.19 & -0.55 & 1 \end{array}\right)$

Table 3 presents a collection of well-known real-world networks with distinct topologies. Our results show that there exists a significant correlation between the symmetry measure δ and the orbit entropy I_a (with a correlation coefficient $R = -0.73$), but does not appear to be correlated with $S(G)$ (with a correlation coefficient $R = -0.15$).

For the networks listed in Table 3, various topological indices, including the first Zagreb index (M_1), second Zagreb index (M_2), spectral radius (ρ), Randic index (R), Laplacian Estrada index (LEE), Laplacian energy (LE), Harary index (H), Estrada index (EE), energy (E), Balaban ID (BI), and atom-bond connectivity (ABC) were calculated, as reported in [1]. The results indicate that among all the above indices, Laplacian energy has the strongest correlation with δ, with a coefficient greater than **0.91**.

$$\left(\begin{array}{c|ccccccccccc} & M_1 & M_2 & \rho & R & LEE & LE & H & EE & E & BI & ABC \\ \hline \delta & -0.07 & 0.47 & -0.19 & -0.17 & -0.02 & \mathbf{0.91} & -0.17 & -0.16 & -0.20 & -0.23 & -0.20 \end{array}\right)$$

For this study, all graphs of orders 4–7, all trees of orders 7–20, together with 470 randomly generated trees of order 21 and 1248 randomly generated trees of order 25 were considered, and two measures based on the automorphism group and Laplacian eigenvalues of a graph were established. The computed correlation values between the unique positive real root δ and Laplacian energy of a graph, denoted by $LE(G)$, are reported in Table 4. For trees of order 21 and 25, the correlation values were 0.556 and 0.589, respectively, whereas for other classes they were less than 0.5.

Although the correlation between δ and $LE(G)$ in real networks is meaningful, it appears that in the class of trees, the correlation value between δ and $LE(G)$ increases as the order of the tree increases. In other words, an appropriate analogy is the case of two functions that have very different functional forms on the same set of variables.

Table 3. A set of well-known real-world networks with distinct topologies and their graph invariants.

Networks	n	δ	M_1	M_2	ρ	R	LEE	LE	H	EE	E	BI	ABC
Human B Cell Genetic	5930	1710×10^{-7}	50,502	63.7×10^{7}	158.8	159.04	-	50.5×10^{3}	40.3×10^{6}	9.48×10^{68}	327.75	-	-
Caenorhabditis elegans Genetic	2060	6258×10^{-7}	13,410	6803	1.62	66.8×10^{2}	56.6×10^{3}	13.3×10^{3}	67.3×10^{2}	20.6×10^{3}	13.3×10^{3}	13,362	66.47
BioGRID Saccharomyccs cerevisiae	5295	1958×10^{-7}	12,032	27.3×10^{5}	1	0.11	142.61	11,998	17	52.46	34	34	1.61
BioGRID Drosophila	7371	1690×10^{-7}	61,434	18.7×10^{7}	2	1.58	224.7	61,410	15	35.21	20	21	4.19
BioGRID Mus musculus	209	$221{,}440 \times 10^{-7}$	18.5×10^{4}	47.3×10^{7}	3.87	1.08	88.9×10^{5}	18.5×10^{4}	89.5	130	51.74	60	9.89
Yeast ProteinInteractions	1458	$11{,}599 \times 10^{-7}$	23,710	19.4×10^{6}	65.75	1076.3	7.11	23.8×10^{3}	61.5×10^{4}	3.60	4141.3	-	4349.1
US Power Grid	4941	2380×10^{-7}	8	16	1	0.25	8.39	6	1	3.09	2	6	0.61
US Airports	332	$40{,}472 \times 10^{-7}$	26,100	14.5×10^{7}	53.51	148.6	7.9×10^{72}	21,947	90,490	1.7×10^{23}	1419	-	-
Email	1133	9216×10^{-7}	10,902	19.7×10^{5}	20.7	460.5	2.54×10^{31}	8399.9	19.2×10^{4}	10.5×10^{8}	2429.9	-	2203.4

Table 4. The correlation values between randomly graphs.

# Graphs	Graph Order	$R(\delta, LE)$
9	2 to 4	−0.414
21	5	−0.009
121	6	0.065
853	7	0.029
33	unicycle graph of order 7	0.031
11	Tree of order 7	0.290
3159	Tree of order 14	0.381
7741	Tree of order 15	0.441
19,320	Tree of order 16	0.429
48,629	Tree of order 17	0.466
123,867	Tree of order 18	0.466
317,955	Tree of order 19	0.493
823,065	Tree of order 20	0.499

5. Small-World Graphs

A social network is called a small-world network, if most nodes are not neighbors of one another, but most nodes can be reached from every other by a small number of hops. The clustering coefficient of a graph is a measure to find which vertices in the graph tend to form a clique. There are two types of clustering coefficient, namely local and global. The local clustering coefficient $C(v)$ of vertex v is defined as $\frac{2e(v)}{d_v(d_v-1)}$, where $e(v)$ is the number of edges $\langle N_G(v)\rangle$. The global clustering coefficient of graph G is $C^{\Delta} = \frac{3t}{l_2}$, where t is the number of triangles and l_2 is the number of paths of length two [25]. Assume that C^{Δ}_{rand} is the clustering coefficient of an equivalent ER random graph with the same order and size. In [25], it is proved that $L_{rand} = \frac{\ln(n)}{\ln(2k)}$ and $C^{\Delta}_{rand} = \frac{2k}{n}$. Additionally, the small-worldness of a graph is expressed by

$$S^{\Delta} = \frac{C^{\Delta}_{g} L_{rand}}{C^{\Delta}_{rand} L_{g}}.$$

Example 3. *Consider three graphs Karate Club $\mathcal{K}$, Dolfin graph $\mathcal{D}$, and the network $\mathcal{G}$, as depicted in Figure 3. The following R programs determine their small-worldness which are, respectively, 1.48, 2. 10, and 4.58.*

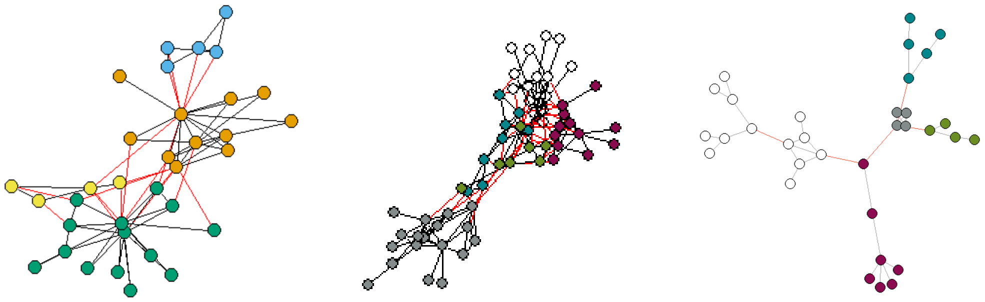

(**a**) Graph $\mathcal{K}$ (**b**) Graph $\mathcal{D}$ (**c**) Graph $\mathcal{G}$

Figure 3. Three small-world graphs (**a**) Karate Club $\mathcal{K}$, (**b**) Dolfin graph $\mathcal{D}$, and (**c**) the network $\mathcal{G}$.

The aim of continuing this paper is to determine whether removing a vertex or an edge decreases or increases the small-worldness of a graph. In the second step, our goal is to determine the small-worldness of two small-world graphs linked by a new edge. To do this, we consider 1000 random small-world networks of the same order. Our results show that by removing a random edge, the resulting graph is again a small-world graph with small-worldness greater than one. We repeated this way by removing a random vertex to conclude a similar result. We applied the following program written by R to obtain our results Algorithm 1.

Algorithm 1: An R program for computing small-worldness of networks

```
library(NetworkToolbox)
library(igraph)
library(Matrix)
count<-0
repeat{
a<-sample(50:60,1)
b<-sample(3:8,1)
g<-sample_smallworld(1,a,b,0.05)
H<-as_adj(g)
L<-matrix(H,nrow=a,ncol=a)
x<-smallworldness(L,method="rand")
p<-sample(V(g),1)
g1<-delete_vertices(g,p)
A<-as_adjacency_matrix(g1)
B<-matrix(A,nrow=a-1,ncol=a-1)
y<-smallworldness(B,method="rand")
t<-cbind(x$swm,y$swm)
write.table(t,file="G-v.csv",append=T,sep=",",col.names=F,row.names=F)
count<-count+1
if(count==1000){break}
}
```

For the second step, we also generate 1000 random small-world graphs joined by a new edge and the resulted graph is again small-world by almost the same small-worldness. The following programs perform this, see Algorithm 2.

To summarize, the results of the investigation indicate that the δ metric is not redundant and offers unique information about the symmetry structure of graphs that cannot be obtained from standard measures, such as small-worldness. Additionally, the successful use of δ as a structural descriptor for chemical structures highlights its potential applications in diverse fields beyond network analysis.

However, further research is necessary to determine the full range of structural properties that can be captured by the orbit polynomial and to better understand the relationship between δ and other graph metrics. Overall, the results suggest that δ is a valuable and versatile tool for analyzing complex systems and may have important implications for a variety of fields.

Algorithm 2: An algorithm for constructing an small-world graph from two small-worled graphs joined by an edge.

```
library(igraph)
library(Matrix)
library(NetworkToolbox)
library(rgl)
count<-0
repeat{
a<-sample(50:100,1)
b<-sample(3:8,1)
g1<-sample_smallworld(1,a,b,0.05)
H<-as_adj(g1)
L<-matrix(H,nrow=a,ncol=a)
x<-smallworldness(L,method=“rand”)
d<-sample(50:100,1)
e<-sample(3:8,1)
g2<-sample_smallworld(1,d,e,0.05)
K<-as_adj(g2)
M<-matrix(K,nrow=d,ncol=d)
y<-smallworldness(M,method=“rand”)
g3<-(g1+g2)%<% add_edegs(c(1,a+d))
A<-as_adjacency_matrix(g3)
B<-matrix(A,nrow=a+d,ncol=a+d)
z<-smallworldness(B,method=“rand”)
write.table(c(x,y,z),file=“new.csv”,append=T,sep=”,”,col.names=F ,row.names=F)
count<-count+1
if(count==1000){break}
}
```

6. Conclusions and Future Work

Counting polynomials, such as the orbit polynomial, play a significant role in the study of real networks due to their ability to systematically analyze network structures, detect symmetries, compare and classify networks, and have algorithmic applications. These polynomials provide insights into the organization, connectivity, and complexity of real networks, enabling researchers to uncover underlying principles and develop efficient algorithms.

Dehmer et al. introduced a novel approach utilizing the modified orbit polynomial and its unique positive real root, δ, to compare graphs based on their symmetry structure. The characteristics of δ have been demonstrated and successfully applied to various network classes to investigate correlations with other graph indices.

Furthermore, the successful application of δ as a structural descriptor for chemical structures is significant as it extends the possibilities of studying symmetry structures in complex systems beyond networks, such as molecules and crystals. This demonstrates the versatility and potential of δ in diverse fields beyond network analysis.

The real positive roots of the modified orbit polynomial have multiple applications in analyzing real networks. They can be employed to detect and study symmetries, automorphisms, and clustering structures within the network. These roots serve as discriminative features in graph isomorphism testing and facilitate comparisons and classifications of different network types. By analyzing the values and patterns of these roots, valuable insights into the structural properties and functional organization of real networks can be obtained.

In conclusion, the orbit polynomial and its associated metric, $\delta(G)$, present a novel approach to compare graphs based on their symmetry structure. Further research is required to comprehensively understand the range of structural properties captured by the orbit polynomial and investigate the relationship between $\delta(G)$ and other metrics, such as the automorphism group index (I_a). This exploration would enhance our understanding of the connection between symmetry and other graph metrics, potentially leading to new insights and applications for δ and related metrics.

This work is subject to certain limitations that merit attention. Firstly, acquiring access to real networks presents a challenge. Furthermore, the employed software restricts the accommodation of trees to a maximum of 26 vertices. Given the overwhelming number of possible graphs surpassing this threshold, executing the program within a polynomial time frame becomes unfeasible. Consequently, the development of novel algorithms for generating trees containing 26 or more vertices becomes imperative, followed by the utilization of these algorithms for subsequent analysis. In essence, the generation of all trees with more than 25 vertices in polynomial time is a computationally arduous undertaking, whereas no specific software capable of efficiently accomplishing this exists; tools such as Cayley, Nauty and Traces, and NetworkX can facilitate the generation of subsets or specific types of trees with enhanced efficiency. It is important to note, however, that the exponential growth in the number of trees poses a significant challenge, rendering the generation of all trees impractical even with the aid of these tools.

Furthermore, we postulate that there exists a relationship between the Pearson correlation of Laplacian energy and δ, and the number of vertices in a tree. Specifically, as the number of vertices increases, we hypothesize that the correlation tends toward 1. The investigation of this relationship between the Pearson correlation of Laplacian energy and δ, and its dependence on the number of vertices in a tree, holds promise as a potential avenue for future research.

Author Contributions: Writing—original draft, R.A.-R. and M.G.; writing—review and editing, M.D. and F.E.-S. All authors have read and agreed to the published version of the manuscript.

Funding: This research received no external funding.

Data Availability Statement: Data sharing not applicable.

Acknowledgments: Modjtaba Ghorbani was partially supported by the Shahid Rajaee Teacher Training University under grant number 5036. Matthias Dehmer thanks the Austrian Science Funds for supporting this work (project P30031). FES would like to thank the Academy of Finland for support (Grant 349043).

Conflicts of Interest: The authors declare no conflict of interest. The funders had no role in the design of the study; in the collection, analyses, or interpretation of data; in the writing of the manuscript; or in the decision to publish the results.

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