



# Article Orbit Polynomial of Graphs versus Polynomial with Integer Coefficients

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**Abstract:** Suppose  $a_i$  indicates the number of orbits of size *i* in graph *G*. A new counting polynomial, namely an orbit polynomial, is defined as  $O_G(x) = \sum_i a_i x^i$ . Its modified version is obtained by subtracting the orbit polynomial from 1. In the present paper, we studied the conditions under which an integer polynomial can arise as an orbit polynomial of a graph. Additionally, we surveyed graphs with a small number of orbits and characterized several classes of graphs with respect to their orbit polynomials.

Keywords: orbit; group action; polynomial roots; orbit-stabilizer theorem



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## 1. Introduction

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 gives 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 [1] of a graph often helps to investigate the structural properties regarding the graph.

Hosoya was the first chemist that introduced the Hosoya counting polynomial (*C*-polynomial) [2] and other well-known *C*-polynomials that have been defined to date, which can be found in references [3–7] as well as [8–11].

One of the important polynomials, as recently defined by Dehmer et al. [12], is the orbit polynomial that uses the cardinalities of the vertex orbit sizes. In the definition of an orbit polynomial, which is  $\sum_{n} cx^{n}$ , c is the number of orbits of graph G of size n. The coefficients of this polynomial are all positive, so subtracting this polynomial from 1 results in the new polyomial  $O_{G}^{*}(x) = 1 - O_{G}(x)$  that has a unique positive root, as can be seen [13–19]. It is possible to define the orbit polynomial for general cases of a graph such as weighted graphs. For instance, for a graph with multiple edges or for a hetero molecule in which an atom is replaced by another, the orbit polynomial can be calculated, as can be seen in [20].

Additionally, in [12], some bounds for the unique and positive zero of  $O_G^*$  were computed. The authors indicated that the unique positive root of this new polynomial can be served as a relative measure of a graph's symmetry. The magnitude of this root measures symmetry and can therefore be used to compare graphs with respect to this property. Finally, it is shown that this measure can be quite useful for tackling applications in chemistry, bioinformatics, and structure-oriented drug design. In [21], the structural attributes of the automorphism group of a graph were investigated, and then the orbit

polynomial of some graph operations were computed. Moreover, the degeneracy of an orbit polynomial is compared with a new counting polynomial. In [22], several properties of orbit polynomial with respect to the stabilizer elements of each vertex and many classes of graphs with a small number of orbits were studied. This method was applied to investigate the symmetry structure of some real-world networks. The main contribution of this text was to construct graphs with a given integer polynomial as its orbit polynomial. We proceed as follows. Section 2 outlines the concepts and definitions that will be used in this paper. In Section 3, we survey some well-known results about the orbit polynomial. In Section 4, we construct graphs whose orbit polynomials are integer and we show that there is a one-to-one correspondence with the number of partitions of an integer *n* and the number of distinct orbit polynomials of a graph of order *n*.

#### 2. Preliminaries

The notations of the current work are standard, for example, as can be seen in [23]. The vertex and edge sets of a graph *G* are denoted by V(G) and E(G), respectively. We only considered simple and connected graphs. The orbit polynomial is based on two concepts: the automorphism group and the vertex orbits.

Consider the automorphism group Aut(G) of graph G. Then, for each vertex  $v \in V(G)$ , the set  $[v] = \{\rho(v) : \rho \in Aut(G)\}$  is called an orbit of G containing v. A vertex-transitive graph is a graph with exactly one orbit and an edge-transitive graph is a graph that is transitive on the set of edges.

The action of group  $\Gamma$  on the set *X* induces a group homomorphism  $\varphi$  from Aut(G) into the symmetric group  $\mathbb{S}_X$  on *X*, where g.x = x for all  $g \in \Gamma$  and  $x \in X$ . For a vertex  $v \in V(G)$ , the set  $S = \{g \in Aut(G) : g(v) = v\}$  is called the stabilizer of *v*. Then, by the orbit-stabilizer theorem, it holds that  $|[v]| \times |S| = |Aut(G)|$ .

The vertex orbits, under the action of automorphisms on the set of vertices, constitutes a partition which captures the symmetry structure of the graph, as can be seen in [13,24–29]. In a complex network, the collections of similar vertices can be used to define communities with shared attributes, as can be seen in [29].

In this paper, the two symbols  $S_n$  and  $B_{n,m}$  denote a star graph on n vertices and a bi-star graph on m + n vertices, respectively. In addition, the graph  $S_{n,m}$  is a tree which has a central vertex of degree n adjacent with n vertices of degree m + 1 each of them is adjacent to m pendant vertices.

## 3. Methods and Results

The orbits of a graph show vertices with similar properties such as having the same degree or the same eccentricity. Conversely, if there exists a property that does not hold for two vertices, then these vertices are not in the same orbit. Thus, creating several kinds of polynomials on the set of orbits of a graph may facilitate distinguishing vertices with different properties and thus breaking them up into distinct orbits.

#### 3.1. Orbit Polynomial

Supposing  $O_1, \ldots, O_t$  are all orbits of *G*. Then, the orbit polynomial and the modified orbit polynomial [13] are defined as

$$O_G(x) = \sum_{i=1}^{t} x^{|O_i|}$$
 and  $O_G^{\star}(x) = 1 - O_G(x)$ .

From the definition, it is clear that if *G* is a graph with an identity automorphism group, then  $O_G(x) = nx$  or equivalently  $O_G^*(x) = 1 - nx$ . Additionally, a graph is only vertex transitive if  $O_G(x) = x^n$ , and only if  $O_G^*(x) = 1 - x^n$ . This means that if *G* and *H* are two vertex-transitive graphs of the same order, then they have the same orbit polynomials  $O_G(x) = O_H(x) = x^n$  and thus the orbit polynomial cannot capture symmetrical information about a vertex-transitive graph, as can be seen in [21].

In algebraic graph theory, characterizing graphs in terms of polynomials such as a characteristic polynomial, independence polynomial, and matching polynomial is always an important problem. Here, we characterize several classes of trees in terms of their orbit polynomial.

**Theorem 1.** *Ref.* [22] *Let T be a tree on n vertices. Then:* 

- $T \cong S_n$  if and only if  $O_T(x) = x + x^{n-1}$ .
- $T \cong B_{\frac{n}{2},\frac{n}{2}}$  if and only if  $O_T(x) = x^2 + x^{n-2}$ .
- $T \cong S_{n,m}$  if and only if  $O_T(x) = x + x^n + x^{nm}$ , where n = 2m.

**Definition 1.** Let  $E_1, \ldots E_r$  be all edge orbits of Aut(G). Then an edge-orbit and the modified edge-orbit polynomials are defined as

$$\widetilde{O}_G(x) = \sum_{i=1}^r x^{|E_i|}$$
 and  $\widetilde{O}_G^*(x) = 1 - \widetilde{O}_G(x)$ .

**Theorem 2.** *Ref.* [22] For the edge-orbit polynomial, we obtain  $\tilde{O}_T(x) = x^{n-1}$  if and only if  $T \cong S_n$ .

As an application, in [22] it was also proven that the cycle graph  $C_n$  can be characterized by the edge version of the orbit polynomial.

#### 3.2. Graph Classification with Respect to Orbit Polynomial

Following the methods of [22], in this section we introduce several classes of graphs that can be characterized by their orbit polynomials. If *G* is a graph with  $O_G(x) = x$ , then clearly  $G \cong K_1$  and, in general, if *G* has *n* vertices and  $O_G(x) = nx$ , then *G* is has no non-identity automorphism. This means that *G* is asymmetric. For a graph with two vertices, it is clear that  $G \cong K_2$  or  $G \cong \overline{K_2}$  and thus  $Aut(G) \cong \mathbb{Z}_2$ . Suppose *G* is a graph with three vertices. Then  $O_G(x) = 3x$  or  $x + x^2$  or  $x^3$ . There is no graph of order 3 with  $O_G(x) = 3x$ , since the smallest graph in the identity automorphism group has at least six vertices, as can be seen in [23]. Graphs with  $O_G(x) = x^3$  are  $K_3$  and its complement and graphs with the orbit polynomial  $O_G(x) = x + x^2$  are  $P_3$  and  $K_1 \cup K_2$ .

There are 11 graphs of order 4 as given in Figure 1. Their orbit polynomials are among the following polynomials:  $O_G(x) = x^4$  or  $O_G(x) = 2x + x^2$  or  $O_G(x) = 2x^2$  or  $O_G(x) = x + x^3$ . According to the above discussion, there is no graph with  $O_G(x) = 4x$ . In addition, there are two graphs with  $O_G(x) = 2x + x^2$ , four graphs with  $O_G(x) = 2x^2$ , two graphs with  $O_G(x) = x + x^3$  and three graphs with  $O_G(x) = x^4$  as given in Figure 1.

For a graph *G* of order *n*, there is a one-to-one correspondence between the possible distinct orbit polynomials and the number of partitions  $\Pi(n)$  of integer *n*. For example, if n = 3, then there are three partitions 3 = 3 and 3 = 1 + 2 and 3 = 1 + 1 + 1 for integer 3 and thus three polynomials  $O_G(x) = x + x + x = 3x$ ,  $O_G(x) = x + x^2$  and  $O_G(x) = x^3$  that can be arisen as orbit polynomials. Since there is no graph of order 3 with the identity automorphism group, all graphs of order 3 have either  $O_G(x) = x + x^2$  or  $O_G(x) = x^3$  as an orbit polynomial. This means that for a graph of order *n*, there are at most  $\Pi(n)$  distinct orbit polynomials. As a result, there are at most 11 distinct polynomials that can be the orbit polynomials of a graph of order 6, since  $\Pi(6) = 11$ . The partitions and correspondence polynomials are reported in Table 1.



Figure 1. All graphs of order 4.

**Table 1.** The partitions and orbit polynomials of all graphs of order 6.

Partition	$O_G(x)$
6 = 6	x <sup>6</sup>
6 = 1 + 5	$x + x^5$
6 = 1 + 1 + 4	$2x + x^4$
6 = 2 + 4	$x^2 + x^4$
6 = 1 + 1 + 1 + 3	$3x + x^3$
6 = 1 + 2 + 3	$x + x^2 + x^3$
3 + 3	$2x^{3}$
6 = 1 + 1 + 1 + 1 + 2	$4x + x^2$
6 = 1 + 1 + 2 + 2	$2x + 2x^2$
6 = 2 + 2 + 2	$3x^2$
6 = 1 + 1 + 1 + 1 + 1 + 1	6 <i>x</i>

Here, we characterize graphs with respect to their orbit polynomials.

**Example 1.** In Figure 2, all members of the class of graphs on six vertices with the orbit polynomial  $O_G(x) = x + x^2 + x^3$  are depicted. They are not isomorphic and have different automorphism groups.



**Figure 2.** All graphs on six vertices with the orbit polynomial  $x + x^2 + x^3$ .

In the next theorem, by  $K_n \bullet re$ , we mean a graph obtained from the complete graph  $K_n$  by attaching *r* pendant edges at a common vertex.

**Theorem 3.** Suppose *G* is a graph with  $O_G(x) = x + x^2 + x^3$ . If *G* has at least a pendant edge, then  $G \cong K_4 \bullet 2e$  or  $G \cong K_3 \bullet 3e$ .

**Proof.** From the definition of an orbit polynomial, we yield that *G* has 6 vertices. As it has exactly one pendant edge, two different singleton orbits, there is a contradiction. Therefore, we may assume that *G* has two pendant edges, then two cases hold: the pendant edges share a common vertex and they necessarily compose an orbit of size 2 and the common vertex composes a singleton orbit. Hence, the other vertices together with the singleton vertex lie on a common 4-cycle. Among all cases, only the graph  $G \cong K_4 \bullet 2e$  satisfies the above conditions. Supposing that the pendant edges have no vertex in common. If two pendant edges can be imaged to each other, since the supported vertices are also in the same orbit, there are at least two orbits of order 2—which is a contradiction. If there are three pendant edges, then *G* is isomorphic with one of the graphs depicted in Figure 3. Among them, only  $G \cong K_3 \bullet 3e$  satisfies the conditions of theorem. This completes the proof.  $\Box$ 



**Figure 3.** All graphs on six vertices that have three pendant edges, with the orbit polynomial  $x + x^2 + x^3$ .

**Example 2.** Consider the graph G with n vertices and suppose that a, b and c are three positive integers that  $1 \le a, b, c \le 3$ . If the orbit polynomial is  $O_G(x) = ax + bx^2 + cx^3$ , then  $O_G(1) = a + 2b + 3c = n$ , and thus  $6 \le n \le 18$ . In Example 1, the problem is solved for n = 6. If n = 7, then we obtain a = 2 and b = c = 1. Hence,  $O_G(x) = 2x + x^2 + x^3$ . Thus, G has two orbits of size 1, an orbit of size 2 and an orbit of size 3. It can be found that there are 39 graphs for this property and we depicted some of them in Figure 4.

If n = 8, then the orbit polynomial of G is either  $O_G(x) = 3x + x^2 + x^3$  or  $O_G(x) = x + 2x^2 + x^3$ . Both cases are possible, as can be seen in Figure 5.

In general, for a graph with  $O_G(x) = ax + x^2 + x^3$ , where a = 1, 2, the orbit-stabilizer theorem yields that 6 = 2.3 | |Aut(G)|. On the other hand, since  $O_G(x) \neq x^6$ , *G* has no permutation of order 6. Similarly, *G* has no permutation of order 4 or 5 and so Aut(G) is a  $\{2,3\}$ -group. This yields that  $|Aut(G)| = 2^{\alpha}.3^{\beta}$ . It holds that |Aut(G)| = 6 or 12 and thus  $Aut(G) \cong \mathbb{Z}_6$  or  $\mathbb{S}_3$  or  $\mathbb{Z}_2 \times \mathbb{S}_3$ . Since *G* has not orbit of size 6, we conclude the following theorem.

**Theorem 4.** 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  $1 \le a, b, c \le 3$ . Then, Aut(G) is a  $\{2,3\}$ -group.

For the automorphism  $g \in Aut(G)$ , the the support of g is defined as  $supp(g) = \{g(u) : u \in V(G)\}$ . Two permutations f and g are said to be disjoint if  $supp(f) \cap supp(g) = \phi$ .



**Figure 4.** Examples of graphs of order 7 with the orbit polynomial  $2x + x^2 + x^3$ .



Figure 5. Graphs of order 8 and different orbit sizes.

**Theorem 5.** *Ref.* [29] *Let S be a set of generators of* Aut(G),  $1 \notin S$  *and*  $S = S_1 \cup ... \cup S_m$ . *Then* 

$$Aut(G) \cong \langle S_1 \rangle \times \langle S_2 \rangle \times \ldots \times \langle S_m \rangle.$$

A network *G* which satisfies Theorem 5 is called locally symmetric. In other words, the network *G* is locally symmetric if Aut(G) can be factorized into a large number of geometric factors.

For a graph  $\Gamma$ , let  $S \subseteq \Gamma$  be a subset of generators of  $\Gamma$ , then  $supp(S) = \bigcup_{s \in S} supp(s)$ .

**Corollary 1.** Let S be a set of generators of Aut(G),  $1 \notin S$  and  $S = S_1 \cup ... \cup S_m$ . Then

$$O_G(x) = tx + \sum_{i=1}^m x^{|supp(s_i)|}$$
 and  $O_G^{\star}(x) = 1 - tx - \sum_{i=1}^m x^{|supp(s_i)|}$ ,

where t is the number of singleton sets.

**Proof.** The structure of the group Aut(G) shows that the elements of each  $supp(s_i)$ ,  $1 \le i \le m$  can be permuted to itself. Hence, the image of elements in  $S_i$ 's are orbits of Aut(G).  $\Box$ 

Suppose A and B are finite groups and B acts on the set X. The wreath product of groups A and B is a group with the underline set:

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

The group operation can be defined as  $(f_1; b_1)(f_2; b_2) = (g; b_1b_2)$ , where for any  $i \in X$ ,  $g(i) = f_1(i)f_2(i^{b_1})$ . For the description of the symmetry of networks, we used the wreath product. For example, suppose  $\mathcal{H}$  is a network constructed from the union of r copies of a graph  $\mathcal{M}$ . Then,  $Aut(\mathcal{H}) \cong S_r \wr Aut(\mathcal{M})$ .

Consider the graph  $\mathcal{G}$  as depicted in Figure 6. It presents a typical arrangement of symmetric subgraphs found in many real-world networks. The structure of the network automorphism group is completely related to the automorphism group of subgraphs induced by its orbits. In [29], the authors determined the structure of the automorphism group of  $\mathcal{G}$ , which is:

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

Hence,  $O_{\mathcal{G}}(x) = 12x + 5x^2 + x^3 + 2x^4$  and  $O_{\mathcal{G}}^{\star}(x) = 1 - (11x + 6x^2 + x^3 + 2x^4)$ .



**Figure 6.** Vertices with the same colors are in the same orbit and singleton orbits are shown by white colors.

## 4. Integer Polynomials

The polynomial  $f(x) = a_0 + a_1x + \dots + a_nx^n$  is called an integer polynomial of degree n, if its coefficients are non-negative integer numbers. The caterpillar tree  $C(n_1, n_2, \dots, n_r)$  is a graph constructed from the path  $P_r$  graph by adding  $n_i$  leafs to the *i*th vertex of  $P_r$ . Consider the caterpillar graph  $G = C(2, 3, \dots, n)$  depicted in Figure 7. Then  $O_G(x) = (n + 4)x + x^2 + \dots + x^n$ .



**Figure 7.** The caterpillar graph G = C(0, 0, 2, 3, ..., n, 0, 0).

It is clear that the orbit polynomial is always a polynomial with integer coefficients, and thus it is an integer polynomial. The aim of this section is to answer the question of whether, supposing  $p(x) = a_0x + a_1x^{n-1} + \ldots + a_kx^{n_k}$  is an integer polynomial, where p(0) = 0, there is any graph whose orbit polynomial is p(x).

**Example 3.** For the caterpillar graph  $\mathcal{G} = C(0, 0, \overbrace{n_1, \cdots, n_1}^{a_1}, \ldots, \overbrace{n_k, \cdots, n_k}^{a_k}, 0, 0)$ , where  $n_i \ge 2$ , we obtain:  $rx + a_1 x^{n_1} + \cdots + a_k x^{n_k}$ ,

where  $r = 4 + \sum_{i=1}^{k} a_i n_i = 4 + k$ .

Here, we determine some classes of graphs with the orbit polynomial  $O_G(x) = \sum_{i=1}^{r} c_i x^{n_i}$ , where r = 1, 2 and  $1 \le c_i \le n$ . If r = 1, then  $O_G(x) = c_1 x^{n_1}$  and thus all orbits of *G* have the same order, namely  $c_1 n_1 = n$  and so  $O_G(x) = c_1 x^{\frac{n}{c_1}}$ . If  $O_G(x) = nx$ , then *G* is the asymmetric graph. For 1 < c < n, let r = n/c, then, the graph  $\mathcal{H} = K_r[rP_c]$  obtained from the complete graph  $K_r$  by attaching the path graph  $P_c$  to each vertex of  $K_r$  (as can be seen in Figure 8), is a graph with the orbit polynomial  $O_G(x) = cx^r$ .



**Figure 8.** The graph  $\mathcal{H} = K_c[nP_r]$ .

In general, we have the following theorem.

**Theorem 6.** Let *G* be a vertex-transitive graph on *n* vertices. Then, the orbit polynomial of graph  $\mathcal{K} = G[nP_k]$  is  $O_{\mathcal{K}}(x) = kx^n$ .

**Proof.** It is clear that all vertices of *G* are in the same orbit. Moreover, the corresponding vertices of each copy of  $P_k$  compose k - 1 orbits of length n.  $\Box$ 

**Theorem 7.** Let G be a graph with two orbits X and Y. Attach to each vertex of X the path graph  $P_k$  and to each vertex of Y, the path  $P_l$ , as can be seen in Figure 9. Then, the resulting graph  $\mathcal{M} = G[P_k, P_l]$  has the orbit polynomial  $O_{\mathcal{M}}(x) = kx^{|X|} + lx^{|Y|}$ .

**Proof.** The proof is straightforward.  $\Box$ 



**Figure 9.** The graph  $\mathcal{M} = G(a_1n_1, \cdots, a_kn_k)$ .

Finally,  $n_i$  ( $n_i$ 's are greater than or equal to zero and at least one of them is not zero) pendent vertices are attached to the *i*th vertex of  $C_k$ . The resulting graph was denoted by

 $C = C_k(\overbrace{n_1, \cdots, n_1}^{a_1}, \cdots, \overbrace{n_k, \cdots, n_k}^{a_k}), \text{ as can be seen in Figure 10. It is not difficult to see that} O_C(x) = kx + a_1x^{n_1} + \cdots + a_kx^{n_k}, \text{ where } |V| = k + n_1 + \cdots + n_k.$ 



**Figure 10.** The graph C.

Thus far, we provided examples of graphs with both polynomials  $O_G(x) = rx + a_1x^{n_1} + \cdots + a_kn_k$  (r = k + 4) and  $O_H(x) = kx + a_1x^{n_1} + \cdots + a_kn_k$ . Thus, for a given integer polynomial  $f(x) = a_1x^{n_1} + \cdots + a_kx^{n_k}$  ( $n_i \ge 2$ ), two polynomials  $O_G(x) = (k + 4)x + f(x)$  and  $O_G(x) = (k)x + f(x)$  are the orbit polynomials of a graph and we conjecture that there is a graph with the orbit polynomial f(x).

#### 5. Summary and Conclusions

In this paper, we investigated the orbit polynomial for several graph/network classes. In addition, we inferred some well-known results about the orbit polynomial. Then, we constructed graphs with a given integer polynomial as its orbit polynomial. The method was applied to investigate the symmetry structure of some real-world networks. Finally, we investigated graphs whose orbit polynomials were integer and we showed that there was a one-to-one correspondence with the number of partitions of an integer n and the number of distinct orbit polynomials of a graph of order n.

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### References

- Hosoya, H. On some counting polynomials in chemistry, Applications of graphs in chemistry and physics. *Discret. Appl. Math.* 1988, 19, 239–257. [CrossRef]
- 2. Hosoya, H. Topological index, a newly proposed quantity characterizing the topological nautre of structural isomers of saturated hydrocarbons. *Bull. Chem. Soc. Jpn.* **1971**, *44*, 2332–2339. [CrossRef]
- 3. Hosoya, H. Clar's aromatic sextet and sextet polynomial. Top. Curr. Chem. 1990, 153, 255–272.
- 4. Farrell, E.J. An introduction to matching polynomials. J. Comb. Theory 1979, 27, 75–86.
- 5. Gutman, I.; Harary, F. Generalizations of the matching polynomial. Util. Math. 1983, 24, 97–106.
- Stevanović, D.; Motoyama, A.; Hosoya, H. King and domino polynomials for polyomino graphs Graph Theory Notes. J. Math. Phys. 1977, 34, 31–36.
- 7. Balasubramanian, K.; Ramaraj, R. Computer generation of king and color polynomials of graphs and lattices and their applications to statistical mechanics. *J. Comput. Chem.* **1985**, *6*, 447–454.
- 8. Farrell, E.J.; De Matas, C.M. On star polynomials of complements of graphs. Ark. Mat. 1989, 26, 85–190. [CrossRef]
- 9. Farrell, E.J.; De Matas, C.M. Star polynomials of some families of graphs with small cyclomatic numbers. *Util. Math.* **1988**, *33*, 33–45.
- 10. Dong, F.M.; Koh, K.M.; Teo, K.L. *Chromatic Polynomials and Chromaticity of Graphs*; World Scientific Publishing Co. Pte. Ltd.: Hackensack, NJ, USA, 2005.
- 11. Balasubramanian, K. On Graph Theoretical Polynomials in Chemistry. In *Mathematical and Computational Concepts in Chemistry*; Trinastić, N., Ed.; Ellis Horwood Ltd.: New York, NY, USA, 1986; pp. 20–33.

- 12. Dehmer, M.; Chen, Z.; Emmert-Streib, F.; Mowshowitz, A.; Varmuzag, K.; Jodlbauer, H.; Shih, Y.; Tripathi, S.; Tao, J. The orbit-polynomial: A novel measure of symmetry in graphs. *IEEE Access* **2020**, *8*, 36100–36112. [CrossRef]
- 13. Dehmer, M.; Chen, Z.; Emmert-Streib, F.; Mowshowitz, A.; Shih, Y.; Tripathi, S.; Zhang, Y. Towards detecting structural branching and cyclicity in graphs: A polynomial-based approach. *Inf. Sci.* **2019**, *471*, 19–28. [CrossRef]
- 14. Dehmer, M.; Shi, Y.; Mowshowitz, A. Discrimination power of graph measures based on complex zeros of the partial Hosoya polynomial. *Appl. Math. Comput.* **2015**, 250, 352–355. [CrossRef]
- 15. Dehmer, M.; Ilić, A. Location of zeros of Wiener and distance polynomials. PLoS ONE 2012, 7, e28328. [CrossRef]
- 16. Ellis-Monaghan, J.A.; Merino, C. Graph polynomials and their applications I: The Tutte polynomial. In *Structural Analysis of Complex Networks*; Dehmer, M., Ed.; Birkhäuser: Boston, MA, USA; Basel, Switzerland, 2010; pp. 219–255.
- 17. Ghorbani, M.; Dehmer, M.; Cao, S.; Tao, J.; Streib, F. On the zeros of the partial Hosoya polynomial of graphs. *Inf. Sci.* **2020**, *524*, 199–215. [CrossRef]
- 18. Tikoo, M.L. Location of the zeros of a polynomial. Am. Math. Mon. 1967, 74, 688–690. [CrossRef]
- 19. Zilovic, M.S.; Roytman, L.M.; Combettes, P.L.; Swamy, M.N. A bound for the zeros of polynomials. *IEEE Trans. Circuits Syst. I* **1992**, *39*, 476–478. [CrossRef]
- 20. Trinajstić, N. Chemical Graph Theory; CRC Press: Boca Raton, FL, USA, 1992.
- 21. Ghorbani, M.; Dehmer, M.; Emmert-Streib, F. On the degeneracy of the orbit polynomial and related graph polynomials. *Symmetry* **2020**, *12*, 1643. [CrossRef]
- 22. Ghorbani, M.; Dehmer, M.; Jalali-Rad, M.; Emmert-Streib, F. Analyzing graphs by means of the orbit polynomial. submitted.
- 23. Harary, F. Graph Theory; Addison-Wesley Publishing Company: Boston, MA, USA, 1969.
- 24. Ghorbani, M.; Dehmer, M.; Rajabi-Parsa, M.; Emmert-Streib, F.; Mowshowitz, A. Hosoya entropy of fullerene graph. *Appl. Math. Comput.* **2019**, 352, 88–98. [CrossRef]
- 25. Ghorbani, M.; Dehmer, M.; Rajabi-Parsa, M.; Mowshowitz, A.; Emmert-Streib, F. On Properties of Distance-Based Entropies on Fullerene Graphs. *Entropy* **2019**, *21*, 482. [CrossRef]
- 26. Ghorbani, M.; Dehmer, M.; Mowshowitz, A.; Emmert-Streib, F. The Hosoya entropy of graphs revisited. *Symmetry* **2019**, *11*, 1013. [CrossRef]
- Mowshowitz, A. Entropy and the complexity of graphs: I. An index of the relative complexity of a graph. *Bull. Math. Biophys.* 1968, 30, 175–204. [CrossRef] [PubMed]
- 28. Mowshowitz, A.; Dehmer, M. The Hosoya entropy of a graph. Entropy 2015, 17, 1054–1062. [CrossRef]
- 29. MacArthur, B.D.; Sánchez-García, R.J.; Anderson, J.W. Symmetry in complex networks. *Disc. Appl. Math.* 2008, 156, 3525–3531. [CrossRef]