Applied Mathematics and Computation 380 (2020) 125239

Contents lists available at ScienceDirect

Applied Mathematics and Computation

journal homepage: www.elsevier.com/locate/amc

Relations and bounds for the zeros of graph polynomials using vertex orbits

Matthias Dehmer[a,b,c,*], Frank Emmert-Streib[d,e], Abbe Mowshowitz[f], Aleksandar Ilić[g], Zengqiang Chen[b], Guihai Yu[j], Lihua Feng[i], Modjtaba Ghorbani[k], Kurt Varmuza[h], Jin Tao[l,m]

[a] Swiss Distance University of Applied Sciences, Department of Computer Science, 3900 Brig, Switzerland
[b] College of Artificial Intelligence, Nankai University, Tianjin 300350, China
[c] Department of Biomedical Computer Science and Mechatronics, UMIT, Hall in Tyrol A-6060, Austria
[d] Predictive Society and Data Analytics Lab, Tampere University, Tampere, Korkeakoulunkatu 10, 33720, Tampere, Finland
[e] Institute of Biosciences and Medical Technology, Tampere University, Tampere, Korkeakoulunkatu 10, 33720, Tampere, Finland
[f] Department of Computer Science, The City College of New York (CUNY), 138th Street at Convent Avenue, New York, NY 10031, USA
[g] Facebook Inc, 1 Hacker Way, Menlo Park, 94025 CA, USA
[h] Institute of Statistics and Mathematical Methods in Economics, Vienna University of Technology, Wiedner Hauptstrasse 7/105-6, Vienna A-1040, Austria
[i] Center for Combinatorics and LPMC, Nankai University, Tianjin 300071, China
[j] School of Mathematics and Statistics, Guizhou University of Finance and Economics, Guiyang, Guizhou 550025, China
[k] Department of Mathematics, Faculty of Science, Shahid Rajaee, Teacher Training University, Tehran 16785-136, I. R., Iran
[l] Department of Electrical Engineering and Automation, Aalto University, Espoo 02150, Finland
[m] College of Engineering, Peking University, Beijing 100871, China

ARTICLE INFO

Article history:
Received 16 January 2020
Revised 13 March 2020
Accepted 16 March 2020

MSC:
62D99
05C75
68R10
90B10

Keywords:
Quantitative graph theory
Networks
Symmetry
Graphs
Graph measures
Data science

ABSTRACT

In this paper, we prove bounds for the unique, positive zero of $O^{\star}_G(z) := 1 - O_G(z)$, where $O_G(z)$ is the so-called orbit polynomial [1]. The orbit polynomial is based on the multiplicity and cardinalities of the vertex orbits of a graph. In [1], we have shown that the unique, positive zero $\delta \leq 1$ of $O^{\star}_G(z)$ can serve as a meaningful measure of graph symmetry. In this paper, we study special graph classes with a specified number of orbits and obtain bounds on the value of δ.

* Corresponding author at: Institute for Intelligent Production, Faculty for Management, University of Applied Sciences Upper Austria, 4040 Steyr, Austria.
E-mail addresses: matthias.dehmer@umit.at (M. Dehmer), frank.emmert-streib@tut.fi (F. Emmert-Streib), abbe@cs.ccny.cuny.edu (A. Mowshowitz), aleksandari@gmail.com (A. Ilić), chenzq@nankai.edu.cn (Z. Chen), yuguihai@126.com (G. Yu), fenglh@163.com (L. Feng), ghorbani30@gmail.com (M. Ghorbani), kurt.varmuza@tuwien.ac.at (K. Varmuza), jin.tao@aalto.fi (J. Tao).

https://doi.org/10.1016/j.amc.2020.125239

1. Introduction

A number of structural graph measures designed to capture symmetry have been developed [1–5]. Most of these measures depend on determining the orbits of the automorphism group of a graph, a task that can be computationally demanding, especially if it is first necessary to compute the automorphism group itself. There is no general formula for the size of the automorphism group of a graph [6,7], and no efficient algorithm for determining the elements of the group. Symmetry is an indicator of structural complexity that can be useful for analyzing graphs. For example, symmetry-based measures have been used to characterize network aesthetics [8]. These measures have also been used to determine the structural complexity of molecules represented by graphs [5]. A shortcoming of symmetry-based measures is the so-called problem of degeneracy [9]. This problem is characterized by the existence of many pairs of non-isomorphic graphs with the same measured value of the index. An attempt to overcome this problem in the case of classical orbit-based entropy measures is presented in [10].

In this paper, we elaborate further on the unique, positive root of the orbit polynomial introduced in [1]. This polynomial is designed as an aid in detecting symmetry in networks. In general, graph polynomials have proven useful in many disciplines such as mathematical chemistry, bioinformatics, and applied mathematics, see [11–14]. In these areas, graph polynomials have been used for counting [13] and also for defining new topological graph measures, see [1,15]. Moreover, well-known graph polynomials such as the chromatic, Tutte, and Jones polynomials have turned out to be useful and important graph invariants for studying problems in applied and pure graph theory, see [16,17].

This paper extends results in [1]. In that earlier paper, we introduced the orbit polynomial $O_G(z)$ and the related graph polynomial $1 - O_G(z)$. The root δ of $1 - O_G(z) = 0$ can be calculated in a straightforward way using a standard root finding method, see [18]. Various properties of δ have been established in [1]. This paper extends the earlier results by proving bounds on δ for graphs with given orbit sizes and multiplicities. Analytical results are given for graphs with two and three orbit sizes and also for more general graphs. In particular, properties of δ are presented for exhaustive sets of isomers of hydrocarbons with 14 carbon atoms. The methods presented here can be applied to any class of graphs.

2. Methods and results

The concept of the *orbit polynomial* was introduced in [1]. In this section we calculate this polynomial for graphs with a given number of vertex orbits [4,19]. Clearly, the number of vertices in each orbit, as well as the multiplicity of orbits of a given cardinality, can vary. In [1], the polynomial $1 - O_G(z)$, derived from the orbit polynomial $O_G(z)$, has been used to measure the symmetry of graphs. The positive zero δ of the polynomial $1 - O_G(z)$ was found to be a useful symmetry measure, see [1].

In short, it is worthwhile to study this algebraic measure because it serves as an index of complexity based on the symmetry structure of a graph. [16]. In this paper, we continue our investigation of the graph measure $\delta \in (0, 1]$ [1], defined as the root of the equation $1 - O_G(z) = 0$. In particular, the measure is applied to graphs whose automorphism group has a specified number of vertex orbits. Since $\delta \in (0, 1]$, we establish lower bounds on δ, as well as other useful properties.

2.1. Preliminaries

This section is devoted to graph-theoretical preliminaries.

An automorphism is an edge preserving bijection of the vertices of a graph [19]. The set of automorphisms under composition of mappings forms the automorphism group of the graph [19] and is usually denoted by Aut(G). $|\mathrm{Aut}(G)|$ is the number of elements in the automorphism group of G. The equivalence classes of the vertices of a graph under the action of the automorphisms are called vertex orbits [19].

Consider a graph $G = (V, E)$ with $|V| < \infty$, and let $V_1, V_2, \ldots, V_\rho$ be its vertex orbits, where ρ denotes the total number of vertex orbits of G. Let k be the number of different cardinalities among the orbit sizes, and suppose the number of orbits of size i_j is $a(i_j)$ for $1 \leq j \leq k$, so that $\sum_{j=1}^{k} i_j a(i_j) = |V|$. $\sum_{j=1}^{k} a(i_j) = \rho$.

For ease of reference, the definitions of orbit polynomial $O_G(z)$ and $1 - O_G(z)$, [1], are reproduced here.

Definition 2.1. The orbit polynomial of G is defined by

$$O_G(z) := \sum_{j=1}^{k} a_{i_j} z^{i_j}. \tag{1}$$

Definition 2.2. The graph polynomial $O_G^{\star}(z)$ of G is defined by

$$O_G^{\star}(z) := 1 - O_G(z). \tag{2}$$

The proof that $\delta \in (0, 1]$ is the unique, positive root of the equation $O_G^{\star}(z) = 0$ and other properties of δ can be found in [1]. Note also that the Definitions (2.1) and (2.2) are valid for directed graphs and edge- or vertex-labeled graphs. Examples of these graphs can be found in [20,21]. For example, the measure δ is directly applicable to molecular graphs [22] possessing different atoms and multiple bonds [21].

2.2. Graphs with two orbits sizes

Here, we investigate δ for graphs with orbits whose size can be of two distinct values. That is to say, the orbits come in two sizes, but there may be several orbits of the same size. The path graph with an odd number of vertices, e.g., $|V| = 5$, is a simple example. Labeling the vertices one to five in sequence starting from one end, the orbits are {1, 5}, {2, 4}, {3}. This graph thus has orbits of two sizes, namely one and two, but the multiplicity of the two-element orbit is two. Obviously, $2 \cdot 2 + 1 \cdot 1 = |V| = 5$.

The following states a lower bound for δ in the case of graphs with two orbit sizes.

Theorem 2.1. *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 δ be the unique, positive root of the equation*

$$O_G^{\star}(\delta) = 1 - (a_{n_1}\delta^{n_1} + a_{n_2}\delta^{n_2}) = 0. \tag{3}$$

Then

$$\delta > \frac{1}{M+1}, \quad \text{where} \quad M := \max\{a_{n_1}, a_{n_2}\}. \tag{4}$$

Proof. In [1], we proved that the unique, positive zero δ of any given $O_G^{\star}(z)$ is less or equal one. Now, we wish to establish a tighter upper bound for δ, where δ is the unique positive root of Eq. (3).

First we find an upper bound for

$$O_G(\delta) = a_{n_1}\delta^{n_1} + a_{n_2}\delta^{n_2}, \tag{5}$$

if $\delta < 1$.

From this we obtain

$$a_{n_1}\delta^{n_1} + a_{n_2}\delta^{n_2} \leq M(\delta^{n_1} + \delta^{n_2}) < M\sum_{j=1}^{\infty}\delta^j = M\left(\frac{1}{1-\delta} - 1\right) = M\frac{\delta}{1-\delta}. \tag{6}$$

Hence

$$a_{n_1}\delta^{n_1} + a_{n_2}\delta^{n_2} < M\frac{\delta}{1-\delta}. \tag{7}$$

Now, we examine the values of δ for which

$$a_{n_1}\delta^{n_1} + a_{n_2}\delta^{n_2} > 1, \tag{8}$$

such that

$$O_G^{\star}(\delta) = 1 - (a_{n_1}\delta^{n_1} + a_{n_2}\delta^{n_2}) < 0. \tag{9}$$

Applying the inequality (7), we find that

$$1 < a_{n_1}\delta^{n_1} + a_{n_2}\delta^{n_2} < M\frac{\delta}{1-\delta}, \tag{10}$$

and, hence,

$$\delta > \frac{1}{M+1}, \tag{11}$$

which completes the proof. □

Consider the path graph P_5 introduced earlier. P_5 has a two-element orbit with multiplicity equal to 2 and a singleton orbit with multiplicity equal to 1. So, we obtain the polynomial

$$O_{P_5}^{\star}(z) = 1 - (2z^2 + z). \tag{12}$$

Calculating the unique, positive root δ of $O_{P_5}^{\star}(z) = 0$ gives $\delta = \frac{1}{2}$. Clearly, $M = 2$. Finally, Theorem (2.1) implies that $\delta > \frac{1}{3}$.

The star graph S_n offers another example. In [1], we proved that $\delta(S_n) \in (0.6823,\ 1), n > 4$, where $\delta(S_n)$ is the unique, positive root of

$$O_{S_n}^{\star}(z) = 1 - O_{S_n}(z) = 1 - (z^{n-1} + z) = 0. \tag{13}$$

Theorem (2.1) implies that $\delta > \frac{1}{2}$.

Theorem 2.2. *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 δ_1 be the zero of Eq. (3) where n_1 and n_2 are fixed, but arbitrary. Assuming n_1 is fixed, but n_2' varies, let δ_2 be the root of the equation*

$$O_G^{\star}(\delta) = 1 - (a_{n_1}{\delta_2}^{n_1} + a_{n_2'}{\delta_2}^{n_2'}) = 0, \tag{14}$$

If $\delta_2 > \delta_1$, then

$$n_2' > \frac{\ln\left(\frac{1-a_{n_1}\delta_1^{\ n_1}}{a_{n_2'}}\right)}{\ln(\delta_1)}. \tag{15}$$

Proof. According to [1], the root of Eq. (3), denoted by δ_1, lies in the interval (0,1]. Now, we locate the root of Eq. (3) when n_1 is fixed but n_2' varies. For this, we calculate

$$O_G^{\star}(\delta_1) = 1 - (a_{n_1}\delta_1^{\ n_1} + a_{n_2'}\delta_1^{\ n_2'}) = -a_{n_1}\delta_1^{\ n_1} - a_{n_2'}\delta_1^{\ n_2'} + 1. \tag{16}$$

If

$$O_G^{\star}(\delta_1) = -a_{n_1}\delta_1^{\ n_1} - a_{n_2'}\delta_1^{\ n_2'} + 1 > 0, \tag{17}$$

then $\delta_2 > \delta_1$. The last inequality also holds as $O_G^{\star}(z)$ is strictly monotonic decreasing. Clearly, the inequality

$$(O_G^{\star}(z))' = -a_{n_1}n_1 z^{n_1-1} - a_{n_2}n_2 z^{n_2-1} < 0, \tag{18}$$

is satisfied for $z > 0$. To calculate n_2', we use Inequality (17). Performing elementary calculations, we obtain Inequality (15). □

To demonstrate Theorem (2.2), we again consider the star graph S_4. According to [1], the positive root of

$$O_{S_4}^{\star}(z) = 1 - (z^3 + z) = 0, \tag{19}$$

is $\delta_1 := \delta(S_4) \doteq 0.682328$. So, $a_{n_1} = a_{n_2} = 1$ and $n_1 = 3, n_2 = 1$. From the second equation

$$O_G^{\star}(z) = 1 - (z^3 + z^2) = 0, \tag{20}$$

we obtain $\delta_2 \doteq 0.754878$. So, $\delta_1 > \delta_2$ and thus $n_2' > 1$, using the given parameters $a_{n_1}, a_{n_2}, n_1, n_2$ in Inequality (15). In fact, $n_2' = 2$.

2.3. Graphs with three orbits sizes

In this section, we study δ for graphs with three orbit sizes, where the multiplicity of orbits of a given size can be greater that one.

The same lower bound as proven in Section (2.2) holds for graphs with three orbit sizes.

Theorem 2.3. *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 δ be the unique, positive root of the equation*

$$O_G^{\star}(\delta) = 1 - (a_{n_1}\delta^{n_1} + a_{n_2}\delta^{n_2} + a_{n_3}\delta^{n_3}) = 0. \tag{21}$$

Then

$$\delta > \frac{1}{M+1}, \quad \text{where} \quad M := \max\{a_{n_1}, a_{n_2}, a_{n_3}\}. \tag{22}$$

Proof. The proof is very similar to the proof of Theorem (2.1).

Now, we prove a result giving the limiting value of the graph measure δ when one orbit size tends to infinity. □

Theorem 2.4. *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 δ be the unique, positive root of the equation*

$$O_G^{\star}(z) = 1 - (a_{n_1}\delta^{n_1} + a_{n_2}\delta^{n_2} + a_{n_3}\delta^{n_3}) = 0. \tag{23}$$

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

$$-a_{n_2}\delta^{n_2} - a_{n_3}\delta^{n_3} + 1 = 0. \tag{24}$$

Proof. Our first observation is

$$O_G^{\star}(z) = 1 - (a_{n_1}\delta^{n_1} + a_{n_2}\delta^{n_2} + a_{n_3}\delta^{n_3}) = -a_{n_1}\delta^{n_1} - a_{n_2}\delta^{n_2} - a_{n_3}\delta^{n_3} + 1 = 0, \tag{25}$$

where n_2 and n_3 are fixed, but arbitrary. Any other combination of the n_i could be chosen as well. Since $\delta \in (0, 1)$,

$$\lim_{n_1\to\infty}(-a_{n_1}\delta^{n_1} - a_{n_2}\delta^{n_2} - a_{n_3}\delta^{n_3} + 1) = 0, \tag{26}$$

becomes

$$-a_{n_2}\delta^{n_2} - a_{n_3}\delta^{n_3} + 1 = 0. \tag{27}$$

Now, define $F(\delta) := -a_{n_2}\delta^{n_2} - a_{n_3}\delta^{n_3} + 1$. Clearly, $F(0) = 1$ and $\lim_{\delta\to\infty}F(\delta) = -\infty$. From Descartes' rule of sign [23], it follows that $F(\delta)$ has a unique, positive zero. In order for $\delta \in (0, 1)$, $F(1) = -a_{n_2} - a_{n_3} + 1 < 0$ must be satisfied; but this is equivalent to $a_{n_2} + a_{n_3} > 1$. This inequality is obviously satisfied. The statement also holds if the orbit sizes are changed so that $n_2 \to \infty$ and $n_3 \to \infty$, instead of $n_1 \to \infty$. □

Theorem 2.5. *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 δ_1 be the zero of Eq. (21) if, for example, n_1, n_2, n_3 are fixed, but arbitrary. Let δ_2 be the root of the equation

$$O^{\star}_G(z) = 1 - (a_{n_1'} {\delta_2}^{n_1'} + a_{n_2} {\delta_2}^{n_1} + a_{n_3} {\delta_2}^{n_1}) = 0, \tag{28}$$

where we assume that n_2, n_3 are fixed but n_1' varies. If $\delta_2 > \delta_1$, then

$$n_1' > \frac{\ln\left(\frac{1 - a_{n_2} {\delta_1}^{n_2} - a_{n_3} {\delta_1}^{n_3}}{a_{n_1'}}\right)}{\ln(\delta_1)}. \tag{29}$$

Proof. According to [1], the root of Eq. (21), denoted by δ_1, lies in the interval (0,1]. Now, we locate the root of Eq. (3), if n_2 and n_3 are fixed but n_1' varies. Clearly, these variables can be interchanged.

Consider

$$O^{\star}_G(\delta_1) = 1 - (a_{n_1'} {\delta_1}^{n_1'} + a_{n_2} {\delta_1}^{n_2} + n_3 {\delta_1}^{n_3}) = -a_{n_1'} {\delta_1}^{n_1'} - a_{n_2} {\delta_1}^{n_2} - n_3 {\delta_1}^{n_3} + 1, \tag{30}$$

and observe that the function

$$O^{\star}_G(z) = -a_{n_1} z^{n_1} - a_{n_2} z^{n_2} - a_{n_3} z^{n_3} + 1, \tag{31}$$

is strictly monotonic decreasing as

$$(O^{\star}_G(z))' = -a_{n_1} n_1 z^{n_1 - 1} - a_{n_2} n_2 z^{n_2 - 1} - a_{n_3} n_3 z^{n_3 - 1} < 0, \tag{32}$$

for $z > 0$.

Combined with the claim

$$O^{\star}_G(\delta_1) = -a_{n_1'} {\delta_1}^{n_1'} - a_{n_2} {\delta_1}^{n_2} - n_3 {\delta_1}^{n_3} + 1 > 0, \tag{33}$$

this implies $\delta_2 > \delta_1$. To establish an inequality for n_1', observe that Inequality (33) holds, which allows for concluding with Inequality (29).

Finally, we show that the numerator of the logarithmic term in the numerator of the right hand side of Inequality (29) is greater than zero. If

$$F(\delta) := -a_{n_1} \delta^{n_1} - a_{n_2} \delta^{n_2} - a_{n_3} \delta^{n_3} + 1, \tag{34}$$

$$F_1(\delta) := -a_{n_2} \delta^{n_2} - a_{n_3} \delta^{n_3} + 1, \tag{35}$$

then

$$F(\delta) < F_1(\delta). \tag{36}$$

As seen in the proof of Theorem (2.4), the zero δ_1 of $F(\delta)$ (also see Eq. (21)) lies between zero and one. It can be shown similarly that the unique, positive root $\delta^{\star}$ of $F_1(\delta)$ also lies between zero and one. Using the technique applied to Eq. (33), as stated above, it follows immediately that $F(\delta)$ and $F_1(\delta)$ are strictly monotonic decreasing for positive δ. From this observation together with Inequality (36), it follows that $\delta_1 < \delta^{\star}$. However, from Inequality (36), we finally obtain

$$F_1(\delta_1) = 1 - a_{n_2} {\delta_1}^{n_2} - a_{n_3} {\delta_1}^{n_3} > 0, \tag{37}$$

which completes the proof. □

2.3.1. Special case of graphs with three orbit sizes

In this section, we investigate δ for graphs with three orbit sizes and given multiplicities.

Although there is no known general method for constructing graphs with prescribed orbit structure (i.e., a given number and specified sizes of the orbits), various heuristics can be used [24]. Perhaps the simplest heuristic is first to build a disconnected graph G with the prescribed orbit structure. The complement of disconnected G is connected and has the same group as G. Suppose, for example, a connected graph with four orbits of sizes 3,4,5,and 6, respectively is wanted. The disconnected graph with pairwise non-isomorphic components G_1, G_2, G_3, and G_4, with vertex sets of sizes 3,4,5,and 6, respectively, whose automorphism groups are transitive provides the requisite orbit structure. Taking the complement of this disconnected graph completes the construction. Among the transitive graphs that could be used in this construction are cycles and complete graphs. A more direct heuristic for building a connected graph with prescribed orbit structure is also given in [24].

Now, we turn to the special case of graphs with three orbits. Consider the graph shown in Fig. (1).One orbit of this graph contains m vertices, the second is a singleton set, and the third contains n vertices, see Fig. (1). The orbit polynomial is easily computed to be

$$O(z) = z^n + z^m + z, \tag{38}$$

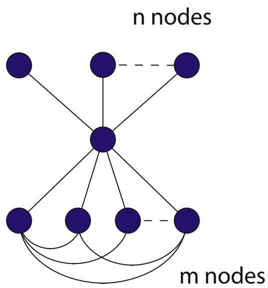

Fig. 1. A graph with three orbits. The first orbit contains m vertices, the second one is a singleton set, and the third contains n vertices.

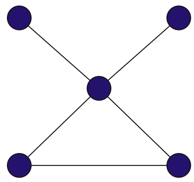

Fig. 2. The graph from Fig. (1) with $m = n = 2$.

and

$$O^{\star}_G(z) = 1 - O_G(z) = 1 - (z^n + z^m + z). \tag{39}$$

First, consider the case $m = n$. This implies

$$O^{\star}_G(z) = 1 - (2z^n + 1) = -2z^n - z + 1. \tag{40}$$

We start by establishing a lower bound for the zero of Eq. (40). An example showing a graph with $m = n = 2$ is presented in Fig. (2).

Theorem 2.6. *Setting $n = m = 2$, we get $\delta^{n=2} = \frac{1}{2}$. This value is a lower bound for all polynomials given by Eq. (40), when $n > 2$.*

Proof. If $n = m = 2$, then

$$O^{\star}_G(\delta) = -2\delta^2 - \delta + 1 = 0. \tag{41}$$

From direct calculations, it is easily seen that this implies $\delta^{n=2} = \frac{1}{2}$. Also, Eq. (40) is strictly monotonic decreasing since

$$(O^{\star}_G(z))' = -2nz^{n-1} - 1 < 0, \tag{42}$$

for $z > 0$. This observation supports the claim that

$$O^{\star}_G(\delta^{n=2}) = -2\left(\delta^{n=2}\right)^n - \delta^{n=2} + 1 > 0. \tag{43}$$

Elementary calculations on Inequality (42) show that

$$n > \frac{\ln\left(\frac{1-\delta^{n=2}}{2}\right)}{\ln\left(\delta^{n=2}\right)}. \tag{44}$$

Substituting $\delta^{n=2} = \frac{1}{2}$ in Inequality (44) shows that $n > 2$. So, $\delta^{n=2} = \frac{1}{2}$ is a lower bound for all polynomials given by Eq. (40). □

Theorem 2.7. *Let $\delta < 1$ be the unique, positive root of the equation*

$$O^{\star}_G(\delta) = -2\delta^n - \delta + 1 = 0. \tag{45}$$

The limiting value of δ is one if n goes to infinity.

Proof. First observe that

$$\lim\,(-2\delta^n - \delta + 1) = -\delta + 1. \tag{46}$$

Clearly, $-\delta + 1 = 0$ implies $\delta = 1$. □

The next theorems improve on the lower bounds.

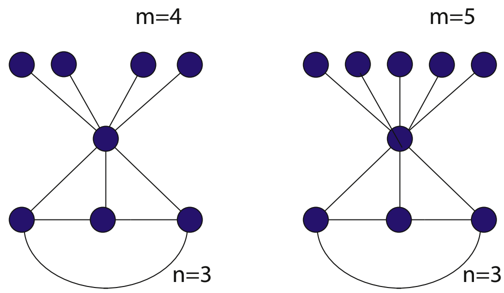

Fig. 3. The graph from Fig. (1) with $m = 4$ and $n = 3$ and $m = 5$ and $n = 3$.

Theorem 2.8. *Let $n = m$. The unique positive root δ of the equation*

$$O^{\star}_{G}(z) = 1 - (2z^{n} + z) = -2z^{n} - z + 1 = 0, \tag{47}$$

satisfies $\delta \geq \frac{1}{3}$.

Proof. The first step in the proof is to give an upper bound for

$$O_{G}(\delta) = 2\delta^{n} + \delta, \tag{48}$$

if $\delta < 1$.

From this we derive

$$2\delta^{n} + \delta < 2(\delta^{n} + \delta) < \sum_{j=1}^{\infty} \delta^{j} = 2\left(\frac{1}{1-\delta} - 1\right) = \frac{2\delta}{1-\delta}. \tag{49}$$

Now consider the values of δ for which

$$2\delta^{n} + \delta > 1, \tag{50}$$

such that

$$1 - (2\delta^{n} + \delta) < 0. \tag{51}$$

Together with Inequality (52), this implies

$$1 < 2\delta^{n} + \delta < \frac{2\delta}{1-\delta}, \tag{52}$$

and, finally,

$$1 < \frac{2\delta}{1-\delta}, \tag{53}$$

Since $\delta < 1$, Inequality (53) gives $\delta > \frac{1}{3}$. Also, if $n = 1$ is chosen for

$$O^{\star}_{G}(\delta) = -2\delta^{n} - \delta + 1 = 0, \tag{54}$$

we get

$$-2\delta - \delta + 1 = 0. \tag{55}$$

This leads to $\delta = \frac{1}{3}$. Using the proof technique of Theorem (2.6), the result of the theorem follows. □

The next assertion deals with the case $n \neq m$. Fig. (3) also shows an example with $m = 5$ and $n = 3$.

Theorem 2.9. *Suppose $n \neq m$. The unique positive root δ of the equation*

$$O^{\star}_{G_{m,n}}(z) = 1 - (z^{n} + z^{m} + z) = -z^{m} - z^{n} - z + 1 = 0, \tag{56}$$

satisfies $\delta \in [\sqrt{2} - 1,\ 1)$ if

$$m > \frac{\ln[1 - (\delta^{\star})^{n} - \delta^{\star}]}{\ln(\delta^{\star})}, \tag{57}$$

where $\delta^{\star} = \sqrt{2} - 1 \doteq 0.41421$ is the unique root of the Eq. (58).

Proof. The simplest case to consider is $m = 2$ and $n = 1$. This gives the equation

$$O^{\star}_{G_{2,1}}(z) = -z^{2} - 2z + 1 = 0, \tag{58}$$

and $\delta^\star = \sqrt{2} - 1 \doteq 0.41421 < 1$. Furthermore, the polynomial represented by the left-hand-side of the Eq. (56) is strictly monotonic decreasing for $z > 0$ because the inequality

$$(O^\star_{G_{m,n}}(z))' = -mz^{m-1} - nz^{n-1} < 0, \tag{59}$$

is satisfied. In order to prove the lower bound, we must determine m (n is fixed) such that

$$O^\star_{G_{m,n}}(z) = -(\delta^\star)^m - (\delta^\star)^n - \delta^\star + 1 > 0. \tag{60}$$

From elementary calculations, we obtain Inequality (57). Now Inequality (57) is a valid expression since $1 - (\delta^\star)^n - \delta^\star > 0$ for $n > \frac{\ln(1-\delta^\star}{\ln(\delta^\star)} \doteq 0.60677$. Let $\delta < 1$ with $\delta > \delta^\star$ be the positive root of the equation

$$O^\star_{G_{m,n}}(\delta) = -\delta^m - \delta^n - \delta + 1 = 0. \tag{61}$$

This implies

$$\lim_{n,m\to\infty}(-\delta^m - \delta^n - \delta + 1) = -\delta + 1 \tag{62}$$

which gives the limiting value $\delta = 1$. □

Theorem (2.9) can be improved by utilizing Bernoulli's inequality [25] to obtain a better upper bound instead of 1. Namely, let's set

$$F(z) = z^m + z^n + z - 1, \tag{63}$$

and, we will prove that $F(y) > 0$ where $y = 1 - \frac{2}{m+n+1}$. By applying Bernoulli's inequality, we conclude

$$\begin{aligned} F\left(1 - \frac{2}{m+n+1}\right) &\geq 1 - \frac{2m}{n+m+1} + 1 - \frac{2n}{n+m+1} + 1 - \frac{2}{m+n+1} - 1 \\ &= 2 - \frac{2m+2n+2}{m+n+1} = 0. \end{aligned} \tag{64}$$

Therefore, we arrived at a better upper bound namely $1 - \frac{2}{m+n+1}$. □

Theorem 2.10. *Suppose $n \neq m$, and consider*

$$O^\star_{G_{m,n}}(z) = 1 - (z^n + z^m + z) = -z^m - z^n - z + 1 = 0. \tag{65}$$

Let δ_1 be the root of Eq. 65 for fixed but arbitrary n and m; and for fixed n but varying m', let δ_2 be the root of equation

$$O^\star_{G_{m,n}}(z) = -z^{m'} - z^n - z + 1 = 0. \tag{66}$$

If $\delta_2 > \delta_1$, then

$$m > \frac{\ln[1 - {\delta_1}^n - \delta_1]}{\ln(\delta_1)}. \tag{67}$$

Proof. By hypothesis,

$$O^\star_{G_{m,n}}(\delta_1) = -{\delta_1}^m - {\delta_1}^n - \delta_1 + 1 = 0. \tag{68}$$

In addition, assume that

$$O^\star_{G_{m,n}}(\delta_2) = -{\delta_2}^{m'} - {\delta_2}^n - \delta_2 + 1 = 0. \tag{69}$$

From the proof of Theorem (2.9), it is clear that $O^\star_{G_{m,n}}(z)$ is strictly monotonic decreasing for $z > 0$. Given this fact together with the assertion

$$O^\star_{G_{m,n}}(\delta_1) = -{\delta_1}^{m'} - {\delta_1}^n - \delta_1 + 1 > 0, \tag{70}$$

it is clear that $\delta_2 > \delta_1$. From Inequality (70) and elementary calculations, we obtain Inequality (67). □

The following is an example of Theorem (2.10) with $m = 4$ and $n = 3$, which gives

$$O^\star_{G_{4,3}}(z) = -z^4 - z^3 - z + 1 = 0. \tag{71}$$

The unique, positive root $\delta_1 \doteq 0.618034$. Substituting this value in Inequality (67), gives $m' > 4$. Suppose, $m' = 5$ and $n = 3$ is fixed. Equation

$$O^\star_{G_{5,3}}(z) = -z^5 - z^3 - z + 1 = 0, \tag{72}$$

implies $\delta_2 \doteq 0.636883$. Thus, $\delta_2 > \delta_1$. The corresponding graphs are shown in Fig. (3).

Now we prove a special case of Theorem (2.9).

Theorem 2.11. *Let $\delta < 1$ be the unique, positive root of Eq. (65). If $m \to \infty$, n fixed, the limiting value of the Eq. (65) is the unique, positive root $\hat{\delta}$ of*

$$F_n(z) = -z^n - z + 1 = 0. \tag{73}$$

Proof. By hypothesis, δ is the unique, positive root of Eq. (65).

Hence,

$$\lim_{m\to\infty} (-\delta^m - \delta^n - \delta + 1) = -\delta^n - \delta + 1. \tag{74}$$

In order to determine δ, it is necessary to calculate the unique, positive root $\hat{\delta}$ such that

$$F_n(\hat{\delta}) = -\hat{\delta}^n - \hat{\delta} + 1 = 0. \tag{75}$$

This completes the proof. □

The following result improves Theorem (2.8).

Theorem 2.12. *Let $n \neq m$. The unique positive root δ of Eq. (65) lies in the interval $(\delta_\star, 1)$, where $\delta_\star$ is the unique, positive root of*

$$-z^m + 2z - 1 = 0, \tag{76}$$

Proof. We need to establish a lower bound for the root of equation

$$O^\star_{G_{m,n}}(\delta) = 1 - (\delta^n + \delta^m + \delta) = -\delta^m - \delta^n - \delta + 1 = 0. \tag{77}$$

First, we give an upper bound for $\delta^m + \delta^n + \delta$ and immediately obtain

$$\delta^m + (\delta^n + \delta) < \delta^m + \left(\frac{1}{1-\delta} - 1\right), \tag{78}$$

by means of an infinite geometric series when $\delta < 1$. Next we turn our attention to the values of δ for which

$$\delta^m + \left(\frac{1}{1-\delta} - 1\right) > 1, \tag{79}$$

such that

$$1 - \left[\delta^m + \left(\frac{1}{1-\delta} - 1\right)\right] < 0. \tag{80}$$

From this it follows that

$$1 < \delta^m + \frac{1}{1-\delta} - 1, \tag{81}$$

or,

$$\delta^m + 2\delta - 1 > 0. \tag{82}$$

So, we have found the value of δ satisfying Inequality (82). Suppose

$$F(\delta) := \delta^m + 2\delta - 1, \tag{83}$$

where $\delta_\star$ with $F(\delta_\star) = 0$ is the lower bound. Now, we prove that $\delta_\star < 1$. Obviously, $F(0) = -1$ and $\lim_{\delta\to\infty} F(\delta) = \infty$, and $F(1) = 2$. So, the root $\delta_\star$ lies between zero and one. To prove uniqueness, we observe that the sequence of coefficients of $F(\delta)$ has exactly one sign change. Descartes' rule of signs [23] implies $F(\delta)$ has a unique, positive zero $\delta_\star$, which concludes the proof. □

Now, we illustrate Theorem (2.12) with an example. Consider

$$O^\star_{G_{3,2}}(z) = 1 - (z^3 + z^2 + z) = -z^3 - z^2 - z + 1 = 0. \tag{84}$$

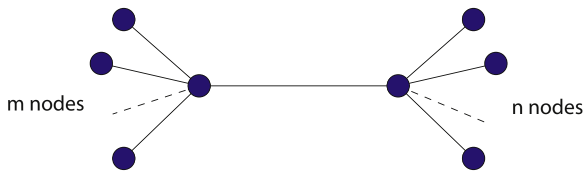

Fig. 4. Another graph with three orbit sizes. We suppose that $n \neq m$. One orbit contains n vertices, the second contains m vertices, and we have two singleton sets.

The real root of Eq. (84) is $\delta \doteq 0.543689$. Theorem (2.8) gives the lower bound $\delta \geq \frac{1}{3}$. In order to determine $\delta_\star$, we need to solve

$$\delta^3 + 2\delta - 1 = 0, \tag{85}$$

which yields $\delta_\star = 0.453398$.

Another example of a graph with three orbits is given in Fig. (4). Compared to the graph shown in Fig. (1), the multiplicity of the singleton orbits is two. So, the associated graph polynomial based on the orbit polynomial is

$$O^{\star,2}_{G_{m,n}}(z) := 1 - (z^n + z^m + 2z) = -z^n - z^m - 2z + 1. \tag{86}$$

To obtain a lower bound in connection with $O^{\star,2}_{G_{m,n}}(\delta) = 0$, we apply Theorem (2.3. This gives $\delta \geq \frac{1}{2+1} = \frac{1}{3}$, as $M = \max\{1, 1, 2\} = 2$. Now it is possible to state a result giving the location of the root δ of $O^{\star,2}_{G_{m,n}}(z)$.

Theorem 2.13. *The unique, positive root of the equation*

$$O^{\star,2}_{G_{m,n}}(z) := 1 - (z^n + z^m + 2z) = -z^n - z^m - 2z + 1 = 0, \tag{87}$$

lies in the interval $\left[\frac{1}{3}, \frac{1}{2}\right)$.

Proof. According to Theorem (2.3), we obtain $\delta \geq \frac{1}{2+1} = \frac{1}{3}$, i.e., $M = 2$. It is clear that the unique, positive root δ is less than one, see Section (2.1). Defining $F(z) := 1 - 2z$ gives

$$O^{\star,2}_{G_{m,n}}(z) = 1 - (z^n + z^m + 2z) < 1 - 2z = F(z), \quad \text{for} \quad z > 0. \tag{88}$$

As demonstrated in the foregoing proofs, we can easily verify that $O^{\star,2}_{G_{m,n}}(z)$ and $F(z)$ are strictly monotonic decreasing for $z > 0$. Also $O^{\star,2}_{G_{m,n}}(0) = F(0) = 1$. Inequality (88) implies that δ is less than the root of $F(z) = 0$. But the root of $F(z) = 0$ equals $z = \frac{1}{2}$. □

As a conclusive remark, we demonstrate that Theorem (2.13) can be slightly improved. Let's define

$$F(z) = z^n + z^m + 2z - 1. \tag{89}$$

So, $F\left(\frac{1}{2}\right) > 0$. By assuming $m \geq n > 2$, we can simply put $y = \frac{1}{2} - \frac{1}{2^n}$. This yields to

$$F(y) = \left(\frac{1}{2} - \frac{1}{2^n}\right)^n + \left(\frac{1}{2} - \frac{1}{2^n}\right)^m + 2\left(\frac{1}{2} - \frac{1}{2^n}\right) - 1 < \frac{1}{2^n} + \frac{1}{2^m} - \frac{1}{2^n} - \frac{1}{2^n} < 0. \tag{90}$$

Therefore, there exists is a root between $\frac{1}{2}$ and $\frac{1}{2} - \frac{1}{2^n}$.

2.3.2. Symmetry of chemical structures

Molecular structures in organic chemistry can be represented as graphs whose vertices denote atoms and whose edges correspond to chemical bonds. Invariants of such graphs, selected from numerical molecular descriptors [5] that have been used successfully in chemoinformatics [26], form groups of topological descriptors. Similarities of chemical structures are defined in terms of sets of descriptors. Furthermore, they serve as variables in multivariate models describing the relationship between chemical structures and substance properties or activities. Such models describe so-called quantitative structure-property (activity) relationships, QSP(A)R. The quantity δ defined above has been proposed as a new topological descriptor characterizing the symmetry of molecular structures.

As an application we calculate δ for three molecular structures to demonstrate the ability of the measure to capture symmetry. The graphs representing these molecular structures are shown in Fig. (5). The relevant polynomials are

$$O^\star_{G_1}(z) = 1 - (z^4 + 4z^2 + 2z), \tag{91}$$

$$O^\star_{G_2}(z) = 1 - (z^6 + z^4 + 2z^2), \tag{92}$$

$$O^\star_{G_3}(z) = 1 - (3z^2 + 8z). \tag{93}$$

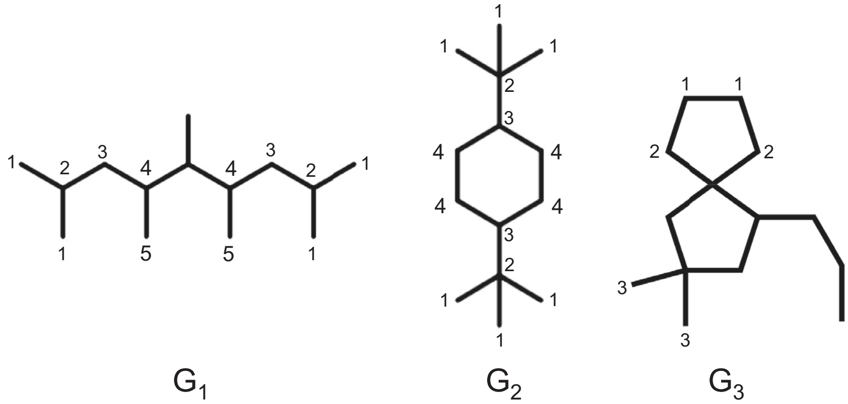

Fig. 5. G_1: An isomer of the set $C_{14}H_{30}$. $\delta(G_1)\doteq0.307026$. G_2: The isomer of the set $C_{14}H_{28}$. $\delta(G_2)\doteq0.626615$. An isomer of the set $C_{14}H_{26}$. $\delta(G_3)\doteq0.119633$. The vertices are labelled by orbit numbers, i.e., a given vertex is in the orbit 1,2,3,4,5. If a vertex is not labeled by this number, then this vertex represents a singleton orbit.

From these we obtain the values $\delta(G_1)\doteq0.307026$, $\delta(G_2)\doteq0.626615$ and $\delta(G_3)\doteq0.119633$. In [1], we analyzed the meaning of the symmetry measures δ and found that the higher the value of δ, the greater is the symmetry of the corresponding graph. Recall that the maximum value of δ is 1, which is achieved in vertex transitive graphs. The following inequalities hold: $\delta(G_2)>\delta(G_1)>\delta(G_3)$. For example, G_2 has a higher degree of symmetry than G_1. This seems to be plausible as G_2 contains at least one ring and G_1 is just a branched path.

From the triangular inequality, we can easily obtain a lower bound for the zeros of the Eqs. (91)–(93). For example, assuming $|z|<1$, the bound on $\delta(G_2)$ is given by

$$\begin{aligned} |O^{\star}_{G_2}(z)| &= |1-(z^6+z^4+2z^2)|, \\ &\geq 1-|z^6+z^4+2z^2|, \\ &\geq 1-\{|z|^6+|z|^4+2|z|^2\}, \\ &\geq 1-2\{|z|^6+|z|^4+|z|^2\}, \\ &\geq 1-2\{3|z|^2\}>0. \end{aligned} \tag{94}$$

So, if $|O^{\star}_{G_2}(z)|>0$, then $|z|<\frac{1}{\sqrt{6}}$. Therefore, all zeros of $O^{\star}_{G_2}(z)$ lie in $|z|\geq\frac{1}{\sqrt{6}}\doteq0.40825$. In fact, $\delta(G_2)\doteq0.626615$.

Now consider δ for hydrocarbons which are essential constituents of mineral oils and other products. These compounds have chemical formulae C_nH_m. A carbon atom (C) has four chemical valences so each vertex of the graph representing it has degree at most four. The maximum number of hydrogen atoms (H) in the compound is $2n+2$, defining the class of alkanes, whose graphs are trees. The different topologies of n connected C-atoms define the set of isomers. In the example presented here, we use graphs with $n=14$ C-atoms (vertices). The number of possible trees (isomers of $C_{14}H_{30}$) is 1858, ranging from the 14-member chain to highly branched graphs; an example is G_1 shown in Fig. (5). The chemical structures are shown in the figure without H-atoms (H-depleted). the numbering of the vertices is arbitrary, and all the edges are identical; such uncolored graphs represent the skeletons of molecular structures. A second set of graphs used here are the isomers derived from $C_{14}H_{28}$, which contain one ring of size ranging from 3 to 14; these cycloalkanes consist of 22,565 isomers. One of the isomers is G_2 shown in Fig. (5). The third set contains the isomers derived from $C_{14}H_{26}$, restricted to structures with two rings with minimum size of 5. These bicycloalkanes consist of 22,314 isomers, one of which is G_3 shown in Fig. (5).

The graphs of the isomeric chemical structures have been generated by the program Molgen [27]; automorphism data has been calculated by software SubMat [28,29].

Table 1 contains the results obtained for the sets of chemical molecular graphs described above. Due to the integer parameters of the orbit polynomials, a discrete set of δ-values appears. The number of different δ-values for each of the three sets is 43, 41 and 36, respectively. These relatively small numbers indicate that δ is a generalized measure for symmetry, rather than a highly unique identifier.

The histograms for the frequencies of the particular δ-values are presented as bar plots in Fig. (6). The distributions for the three sets appear similar with high frequencies at low symmetry; the medians are 0.09808, 0.098080 and 0.08276.

The minimum value of δ, δ_{min}, for a graph with n vertices (C-atoms here) occurs for asymmetric graphs having each atom in a separate orbit.In this case the atoms are all topologically different. The polynomial is $1-nz$ and $\delta_{\text{min}}=\frac{1}{n}$; here $\frac{1}{14}=0.07143$. For each set of isomeric structures the δ_{min} is equal to this theoretical minimum; the number of asymmetric graphs is 139, 3028 and 8785, respectively, for the three sets. Examples are presented in Fig. (7).

The maximum value of δ, δ_{max}, for a graph with n vertices (C-atoms here) is obtained if all atoms are in a single orbit, in which case the atoms all topologically equal. The polynomial is $1-z^n$ and $\delta_{\text{max}}=1$. Such a graph exists in set 2

Table 1
Data sets from chemical structures with 14 carbon atoms and automorphism parameter.

	Set 1	Set 2	Set 3
Chemical formula	$C_{14}H_{30}$	$C_{14}H_{28}$	$C_{14}H_{26}$
No. of rings	0	1	2
No. of isomeric structures	1858	22,565	22,314
δ_{min}	0.07143	0.07143	0.07143
δ_{median}	0.09808	0.09808	0.08276
δ_{max}	0.76795	1.00000	0.76795
No. of unique δ	43	41	36
No. of structures with δ_{min}	139	3028	8785
No. of structures with δ_{max}	1	1	2
$\|Aut(G)\|$ range	1–1296	1–288	1–48
No. of structures with max($\|Aut(G)\|$)	1	1	4

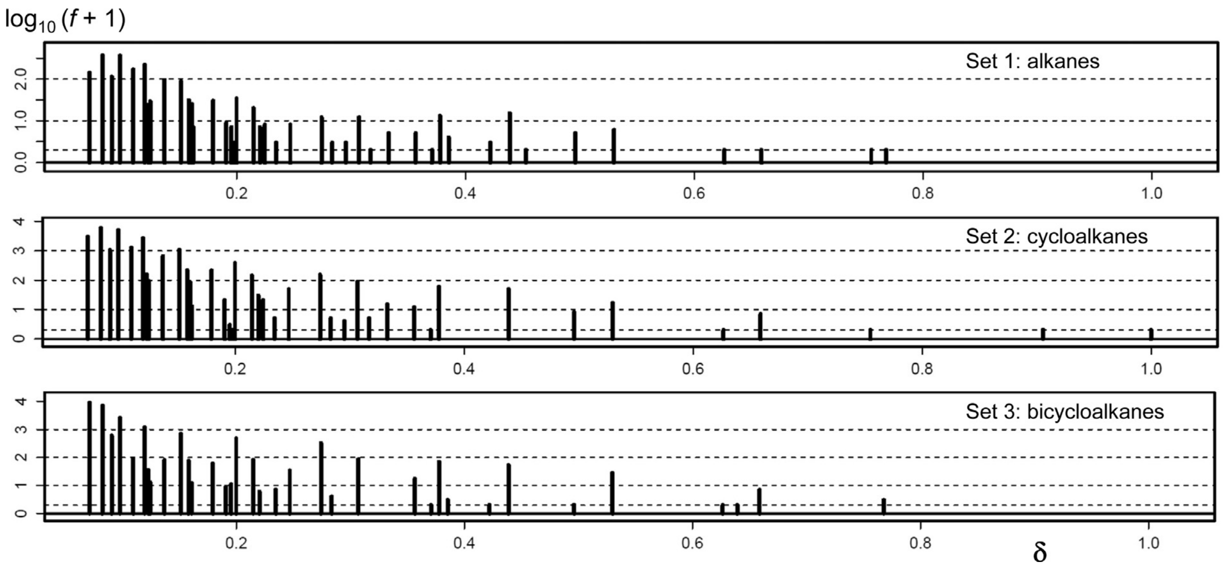

Fig. 6. Distribution of the δ-values for the three sets containing chemical structures. The frequency, f, is plotted as $\log_{10}(f+1)$.

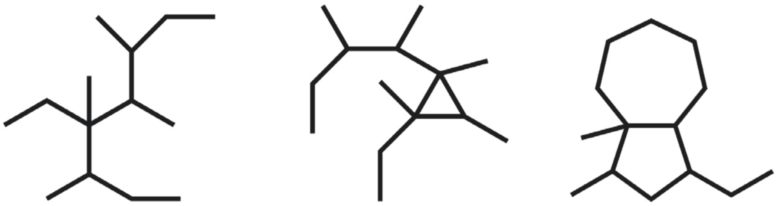

Fig. 7. Examples of asymmetric graphs for the three sets with chemical structure graphs, all with the theoretical minimum of δ for 14 vertices. $\delta_{min} = \frac{1}{14} = 0.07143$.

(cycloalkanes), consisting of a 14-member ring. In set 1 (alkanes) $\delta_{max} = 0.76795$ for one graph; in set 2 (bicycloalkanes) with the same δ_{max} for two graphs; in Fig. 8 these three graphs are presented. All three have 1 orbit with 2 atoms, and 2 orbits with 6 atoms, giving the polynomial $1 - 2z - 2z^6$, with identical δ values for symmetry, despite different visual impressions of the molecular skeletons.

The orbit data - defining the symmetry measure δ - can be obtained from the automorphism group of the graph, consisting of all possible bijective, edge preserving mappings of the vertices. The size, $|Aut(G)|$, of the automorphism group of an asymmetric graph G (see Section 2.1) is one. Here $\delta_{min} = \frac{1}{n}$. However, in the three sets, the numerical relationship between δ and $|Aut(G)|$ is weak with Pearson correlation coefficients of 0.33, 0.45, and 0.50, respectively. The maximum values of

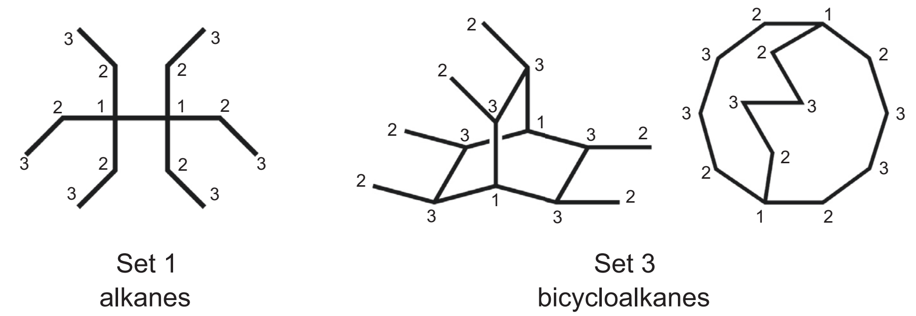

Fig. 8. Graphs with highest $\delta = 0.76795$ in the sets with chemical structure graphs for alkanes (set 1) and bicycloalkanes (set 3). The vertices are labeled by orbit numbers, i.e., a given vertex is in the orbit 1,2,3.

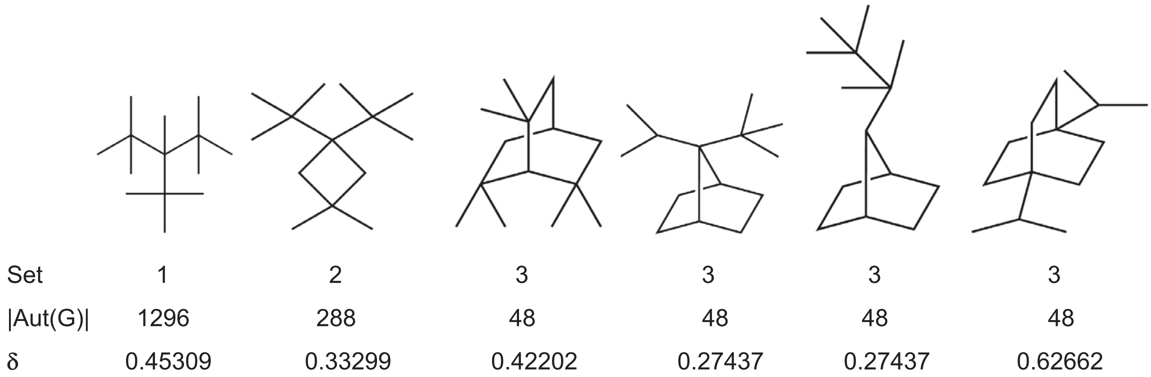

Fig. 9. Graphs with highest size of the automorphism group, $|\mathrm{Aut}(G)|$, in the three sets with chemical structure graphs.

$|\mathrm{Aut}(G)|$ in the three sets are 1296, 288, and 48, respectively; the number of graphs with maximum $|\mathrm{Aut}(G)|$ in the three sets is 1, 1, and 4. Fig. 9 shows these six structures.

3. Summary and conclusion

This paper has addressed the problem of determining bounds on the unique positive roots of certain graph polynomials. These polynomials capture the orbit structure of the automorphism group of a graph, and as such give information about symmetry. The results suggest that the roots of these polynomial can be used to classify graphs according to degree of symmetry. Specific bounds have been given for several classes of graphs. Also, we applied the measures δ to special sets of isomers. The results revealed that the measure captures symmetry meaningfully, however δ shows a certain kind of degeneracy for these sets. We could overcome this problem by defining an appropriate super index. Also, we plan to extend these results to other classes of graphs and to build a foundation for classification.

Acknowledgments

Matthias Dehmer thanks the Austrian Science Fund for supporting this work (project P30031).

Zengqiang Chen was supported by National Natural Science Foundation of China (No. 61573199). Jin Tao was supported by Academy of Finland (No. 315660).

Modjtaba Ghorbani was supported by the Shahid Rajaee Teacher Training University under grant No. 22126.

References

[1] M. Dehmer, Z. Chen, F. Emmert-Streib, A. Mowshowitz, K. Varmuza, L. Feng, H. Jodlbauer, Y. Shi, J. Tao, The orbit-polynomial: a novel measure of symmetry in networks, IEEE Access 8 (2020) 36100–36112, doi:10.1109/ACCESS.2020.2970059.
[2] D. Bonchev, Information Theoretic Indices for Characterization of Chemical Structures, Research Studies Press, s, 1983.
[3] S.C. Basak, A.T. Balaban, G.D. Grunwald, B.D. Gute, Topological indices: their nature and mutual relatedness, J. Chem. Inf. Comput. Sci. 40 (2000) 891–898.
[4] A. Mowshowitz, Entropy and the complexity of the graphs i: an index of the relative complexity of a graph, Bull. Math. Biophys. 30 (1968) 175–204.
[5] R. Todeschini, V. Consonni, Handbook of Molecular Descriptors, Wiley-VCH, Weinheim, Germany, 2002.
[6] C.J. Colbourn, K.S. Booth, Linear time automorphism algorithms for trees, interval graphs, and planar graphs, SIAM J. Comput. 10 (1981) 203–225.
[7] M. Razinger, K. Balasubramanian, M.E. Munk, Graph automorphism perception algorithms in computer-enhanced structure elucidation, J. Chem. Inf. Comput. Sci. 33 (1993) 197–201.

[8] Z. Chen, M. Dehmer, F. Emmert-Streib, A. Mowshowitz, Y. Shi, Toward measuring network aesthetics based on symmetry, Axioms 6 (2017).
[9] E.V. Konstantinova, The discrimination ability of some topological and information distance indices for graphs of unbranched hexagonal systems, J. Chem. Inf. Comput. Sci. 36 (1996) 54–57.
[10] A. Mowshowitz, M. Dehmer, A symmetry index for graphs, Symmetry 21 (4) (2010) 321–327.
[11] B. Jackson, Zeros of chromatic and flow polynomials of graphs, J. Geom. 76 (2003) 95–109.
[12] B.E. Sagan, Y.N. Yeh, P. Zhang, The wiener polynomial of a graph, Int. J. Quant. Chem. 60 (1996) 959–969.
[13] H. Hosoya, On some counting polynomials, Discret. Appl. Math. 19 (1988) 239–257.
[14] P. Křivka, N. Trinajstić, On the distance polynomial of a graph, Appl. Math. 28 (1983) 357–363.
[15] M. Dehmer, M. Moosbrugger, Y. Shi, Encoding structural information uniquely with polynomial-based descriptors by employing the Randić matrix, Appl. Math. Comput. 268 (2015) 164–168.
[16] Y. Shi, M. Dehmer, X. Li, I. Gutman, Graph Polynomials, Wiley-VCH, 2017.
[17] J.A. Ellis-Monaghan, C. Merino, Graph polynomials and their applications I: the Tutte polynomial, in: M. Dehmer (Ed.), Structural Analysis of Complex Networks, Birkhäuser, Boston/Basel, 2010, pp. 219–255.
[18] M. Mignotte, D. Stefanescu, Polynomials: An Algorithmic Approach, Discrete Mathematics and Theoretical Computer Science, Springer, 1999**.** Singapore
[19] C. Godsil, G. Royle, Algebraic Graph Theory, Graduate Texts in Mathematics, Academic Press, 2001.
[20] A. Mowshowitz, Entropy and the complexity of graphs II: the information content of digraphs and infinite graphs, Bull. Math. Biophys. 30 (1968) 225–240.
[21] N. Trinajstić, Chemical Graph Theory, CRC Press, Boca Raton, FL, USA, 1992.
[22] D. Bonchev, D.H. Rouvray, Complexity in Chemistry, Biology, and Ecology, Mathematical and Computational Chemistry, Springer, New York, NY, USA, 2005.
[23] M. Marden, Geometry of Polynomials, Mathematical Surveys of the American Mathematical Society, 3, 1966**.** Rhode Island, USA
[24] A. Mowshowitz, M. Dehmer, F. Emmert-Streib, A note on graphs with prescribed orbit structure, Entropy 21 (11) (2019).
[25] P. Cerone, S.S. Dragomir, Mathematical Inequalities, CRC Press, Boca Raton, FL, USA, 2010.
[26] J. Gasteiger, T. Engel, Chemoinformatics - a Textbook, Wiley VCH, Weinheim, Germany, 2003.
[27] A. Kerber, R. Laue, M. Meringer, C. Rücker, Molecules in silico: a graph description of chemical reactions, J. Chem. Inf. Model. 47 (2007) 805–817.
[28] K. Varmuza, H. Scsibrany, Substructure isomorphism matrix, J. Chem. Inf. Comput. Sci. 40 (2000) 308–313.
[29] K. Varmuza, W. Demuth, M. Karlovits, H. Scsibrany, Binary substructure descriptors for organic compounds, Croat. Chem. Acta 78 (2005) 141–149.