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On the Wiener-like root-indices of graphs

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Abstract
In this paper, we examine roots of graph polynomials where those roots can be considered as structural graph measures. More precisely, we prove analytical results for the roots of certain modified graph polynomials and also discuss numerical results. As polynomials, we use, e.g., the Hosoya, the Schultz, and the Gutman polynomial which belong to an interesting family of degree-distance-based graph polynomials; they constitute so-called counting polynomials with non-negative integers as coefficients and the roots of their modified versions have been used to characterize the topology of graphs. Our results can be applied for the quantitative characterization of graphs. Besides analytical results on bounds and convergence, we also investigate other properties of those measures such as their degeneracy which is an undesired aspect of graph measures. It turns out that the measures representing roots of graph polynomials possess high discrimination power on exhaustively generated trees, which outperforms standard versions of these indices. Furthermore, a new measure is introduced that allows us to compare different topological indices in terms of structure sensitivity and abruptness.

Keywords (Edge-)Hosoya polynomial · Schultz polynomial · Gutman polynomial · Root-index · Discrimination power · Structure sensitivity

Mathematics Subject Classification 05C09 · 05C31 · 05C12 · 05C92 · 40A05 · 92E10

1 Introduction

In network theory and mathematical chemistry, topological indices (Todeschini and Consonni 2002) have been used to quantitatively describe the structure of graphs. In chemistry, they are used in the development of quantitative structure-activity relationships (QSAR) and quantitative structure–property relationships (QSPR) in which some properties of compounds are correlated with their chemical structure (Devillers and Balaban 1999). The origin of this research field goes 75 years back when the famous Wiener index was introduced, see Wiener (1947). The Wiener index has been used in graph theory (Klavžar et al. 1996) as well as in drug design and related fields such as computational chemistry (Basak et al. 2000). Later, several other distance-based indices were invented, for example the edge-Wiener index, which

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was introduced in the same year by Dankelmann et al. (2009); Iranmanesh et al. (2009), and Khalifeh et al. (2009). Moreover, the Schultz index (also known as the degree distance) was firstly introduced in 1994 (Dobrynin and Kochetova 1994). However, a similar concept was invented five years earlier by Schultz (1989). In addition, the Gutman index was also defined in 1994 (Gutman 1994).

Another categorization of graph measures is given in Emmert-Streib and Dehmer (2011) that distinguishes between several categories. In this paper, we consider graph measures which are based on graph polynomials. The concept of using the roots of graph polynomials as structural descriptors has been explored for decades, particularly in the study of graph eigenvalues. One well-known example is the spectral radius, defined as the largest eigenvalue of a (molecular) graph. Notably, strong correlations have been observed between the spectral radius and the Wiener index in the case of alkanes and benzenoid molecules (Radenković and Gutman 2008). On the other hand, Dehmer et al. (2010) contributed to this line of research by defining a special graph polynomial and use the moduli of the zeros of the underlying graph polynomial as graph measures; it turned out that these measures have low degeneracy. After this, Dehmer et al. (2020a) defined the so-called orbit polynomial where it's coefficients are based on vertex orbit cardinalities and proved several properties and bounds thereof, see also Dehmer et al. (2020b). In fact, the orbit polynomial has been used as an efficient symmetry measure for graphs (Ma et al. 2021). Moreover, in Ghorbani et al. (2021) the authors studied the conditions under which an integer polynomial can arise as an orbit polynomial of a graph. Other contributions of Dehmer et al. who started the research on this topic can be found in Dehmer et al. (2015). Some recent contributions to this field are due to Ghorbani et al., in which the authors compared the roots of the modified orbit polynomial with other graph measures (Ghorbani et al. 2023), studied the structure of well-known real-world networks in terms of the orbit polynomial (Ghorbani and Dehmer 2021), and considered the roots of some distance-based graph polynomials (Ghorbani et al. 2022). Furthermore, Brezovnik et al. (2023) examined some measures based on roots of the modified Szeged and Mostar polynomials. Very recently, Zagreb-root indices were introduced and some chemical applications of root-indices in general were investigated (Tratnik and Žigert Pleteršek 2024). In particular, it was shown that Wiener-like root-indices have very high correlations with the following properties of octane isomers: entropy, enthalpy of vaporization, standard enthalpy of vaporization, acentric factor.

As already mentioned, there exist several approaches to define structural graph measures which are based on graph polynomials.

The motivation to define those graph measures (indices) has been multifaceted: one aim has been to derive measures having useful properties such as high discrimination power (Dehmer et al. 2010), correlation ability and/or a meaningful structural interpretation, e.g., symmetry (Dehmer et al. 2020a). Another motivation has been to develop a mathematical apparatus that has strong links to algebra and algebraic graph theory.

Mathematically seen, those measures have been pretty interesting as they are based on algebraic quantities such as zeros of polynomials, but nevertheless captures structural properties of graphs meaningfully. Following the ground breaking work on the so-called orbit polynomial (Dehmer et al. 2020a), it is natural and logical to use the main idea (see Lemma 7 in the present paper) to define other polynomial-based measures. Therefore, we continue this line of research with the investigation of some new graph measures based on certain roots of graph polynomials resulting in the Wiener root-index, the edge-Wiener root-index, the Schultz root-index, and the Gutman root-index. These roots are positive, real-valued and lie in the interval $(0, 1]$. It's evident that they have a certain structural interpretation when measuring the complexity of graphs quantitatively. As already mentioned, a well-known example is the unique, positive root $\delta \in (0, 1]$ of the modified orbit polynomial which has been proven useful as a symmetry measure. In order to define and examine new root-based measures (so-called root-indices), we here focus on the Hosoya polynomial (Hosoya 1988), the edge-Hosoya polynomial (Behmaram et al. 2011), the Schultz polynomial (Gutman 2005), and the Gutman polynomial (Gutman 2005).

In this paper, we explore properties such as bounds of these measures in order to get a better understanding of these quantities and to use them in practice. Investigating these properties is significant, otherwise they cannot be compared with other measures. A further problem of all graph measures relates to shed light on their structural interpretation. This problem has been crucial as the structural interpretation is not yet understood. They have just been used as mathematical quantities.

The paper is organized as follows: we firstly consider closed formulas for the mentioned polynomials of some well-known deterministic graph classes. Then, bounds for the roots of the modified versions of considered polynomials are proved. In addition, convergence of sequences of root-indices is studied. Next, we compute various measures for evaluating the quality of different topological indices. In particular, we consider the discrimination power of root-indices and compare their performance with that of existing similar indices. Next, we consider correlations between different pairs of root-indices and also correlations between them and their standard versions. This analysis reveals interesting links to other existing graph measures. Finally, we investigate structure sensitivity and abruptness which measure how a gradual change of a graph results on the topological index. It is preferred that the first one is as large as possible and the second as small as possible. Therefore, we introduce a new measure SA as their quotient, which enables us to efficiently compare different topological indices.

2 Preliminaries

Let G be a connected graph with at least one edge. Moreover, denote by $d(a, b)$ the standard shortest-path *distance* between vertices $a, b \in V(G)$. In addition, let $\deg(a)$ be the *degree* of vertex a. The distance $d(e_1, e_2)$ between edges e_1 and e_2 of graph G is the distance between the corresponding vertices e_1 and e_2 in the line graph $L(G)$ of G.
The *Hosoya polynomial* (Hosoya 1988) of a graph G, denoted as $H(G, x)$, and the *edge-Hosoya polynomial* (Behmaram et al. 2011) of G, denoted as $H_e(G, x)$, are defined as

$$H(G, x) = \sum_{\substack{\{a,b\}\subseteq V(G)\\ a\neq b}} x^{d(a,b)},$$

$$H_e(G, x) = \sum_{\substack{\{e,f\}\subseteq E(G)\\ e\neq f}} x^{d(e,f)}.$$

If G has only one edge, we define $H_e(G, x) = 0$. Note that usually these polynomials include a nonzero constant term (the number of vertices in the Hosoya polynomial and the number of edges in the edge-Hosoya polynomial). However, the original definition of the Hosoya polynomial does not consider pairs of vertices $\{a, b\}$ in which $a = b$. We use the latest definition since it is more suitable for our purposes.

It is clear that

$$H_e(G, x) = H(L(G), x),$$

where $L(G)$ is the line graph of G.

Moreover, the *Schultz polynomial* (Gutman 2005) of G, denoted as $Sc(G, x)$, and the *Gutman polynomial* (Gutman 2005) of G, denoted as $Gut(G, x)$, are defined as

$$Sc(G, x) = \sum_{\substack{\{a,b\} \subseteq V(G) \\ a \neq b}} (\deg(a) + \deg(b)) x^{d(a,b)},$$

$$Gut(G, x) = \sum_{\substack{\{a,b\} \subseteq V(G) \\ a \neq b}} \deg(a) \deg(b) x^{d(a,b)}.$$

Obviously, the *Wiener index* (Wiener 1947), the *edge-Wiener index* (Dankelmann et al. 2009; Iranmanesh et al. 2009; Khalifeh et al. 2009), the *Schultz index* (Dobrynin and Kochetova 1994; Schultz 1989), and the *Gutman index* (Gutman 1994) can be computed from the mentioned polynomials by evaluating their first derivatives at $x = 1$:

$$W(G) = H'(G, 1), \quad W_e(G) = H_e'(G, 1),$$
$$Sc(G) = Sc'(G, 1), \quad Gut(G) = Gut'(G, 1).$$

Finally, we show an alternative way for writing the polynomials defined above. For a graph G and $k \geq 1$, we define the following sets of unordered pairs of vertices and edges of G:

$$V_k(G) = \{\{a, b\} \subseteq V(G) \mid d(a, b) = k\},$$
$$E_k(G) = \{\{e, f\} \subseteq E(G) \mid d(e, f) = k\}.$$

In addition, for every $k \geq 1$ we set

$$d_k(G) = |V_k(G)|,$$
$$d_k^e(G) = |E_k(G)|,$$
$$s_k(G) = \sum_{\{a,b\} \in V_k(G)} (\deg(a) + \deg(b)),$$
$$g_k(G) = \sum_{\{a,b\} \in V_k(G)} \deg(a) \deg(b).$$

Note that if $V_k(G)$ is an empty set for some $k \geq 1$, then we define $s_k(G) = g_k(G) = 0$.

It is straightforward to see that the following holds:

$$H(G, x) = \sum_{k \geq 1} d_k(G) x^k, \quad H_e(G, x) = \sum_{k \geq 1} d_k^e(G) x^k,$$
$$Sc(G, x) = \sum_{k \geq 1} s_k(G) x^k, \quad Gut(G, x) = \sum_{k \geq 1} g_k(G) x^k.$$

The following numbers will be used in Sect. 4:

$$MH(G) = \max\{d_k(G) \mid k \geq 1\}, \quad MH_e(G) = \max\{d_k^e(G) \mid k \geq 1\},$$
$$MS(G) = \max\{s_k(G) \mid k \geq 1\}, \quad MG(G) = \max\{g_k(G) \mid k \geq 1\}.$$

3 Explicit formulas for some degree-distance-based polynomials

Here we state the explicit formulas for the Hosoya polynomial, the edge-Hosoya polynomial, the Schultz polynomial, and the Gutman polynomial for some families of graphs. It should be pointed out that some of the results are quite straightforward and were already stated in earlier papers, for example see Behmaram et al. (2011).

Proposition 1 *For the complete graph K_n with n vertices, $n \geq 1$, it holds*

$$\begin{aligned} H(K_n, x) &= \frac{n(n-1)}{2}x, \\ Sc(K_n, x) &= n(n-1)^2 x, \\ Gut(K_n, x) &= \frac{n(n-1)^3}{2}x. \end{aligned}$$

Proposition 2 *For the complete graph K_n with n vertices, $n \geq 1$, it holds*

$$H_e(K_n, x) = \frac{n^3 - 3n^2 + 2n}{2}x + \frac{n^4 - 6n^3 + 11n^2 - 6n}{8}x^2.$$

Proof It can be easily checked that the formula holds for $n = 2$ and $n = 3$. Therefore, let $n \geq 4$. If two distinct edges $e = ab$ and $f = uv$ of K_n are not adjacent, then $d(e, f) = 2$ since for example bu is an edge in K_n. Consequently, the diameter of $L(K_n)$ equals two.

Moreover, every edge of K_n is adjacent to exactly $2(n-2)$ other edges, and therefore, the number of pairs of edges at distance one is

$$\frac{\binom{n}{2}2(n-2)}{2} = \frac{n^3 - 3n^2 + 2n}{2}.$$

Hence, the number of pairs of edges at distance two is

$$\binom{\binom{n}{2}}{2} - \frac{n^3 - 3n^2 + 2n}{2} = \frac{n^4 - 6n^3 + 11n^2 - 6n}{8},$$

which completes the proof. □

Proposition 3 *For the cycle C_n with n vertices, $n \geq 3$, it holds*

$$H(C_n, x) = H_e(C_n, x) = \begin{cases} nx\left(1 + x + \cdots + x^{\frac{n}{2}-2} + \frac{1}{2}x^{\frac{n}{2}-1}\right); & n \text{ even} \\ nx\left(1 + x + \cdots + x^{\frac{n-3}{2}}\right); & n \text{ odd} \end{cases},$$

$$Sc(C_n, x) = Gut(C_n, x) = \begin{cases} 4nx\left(1 + x + \cdots + x^{\frac{n}{2}-2} + \frac{1}{2}x^{\frac{n}{2}-1}\right); & n \text{ even} \\ 4nx\left(1 + x + \cdots + x^{\frac{n-3}{2}}\right); & n \text{ odd} \end{cases}.$$

Proposition 4 *For the star S_n with $n + 1$ vertices, $n \geq 1$, it holds*

$$\begin{aligned} H(S_n, x) &= nx + \frac{n(n-1)}{2}x^2, \\ Sc(S_n, x) &= n(n+1)x + n(n-1)x^2, \\ Gut(S_n, x) &= n^2 x + \frac{n(n-1)}{2}x^2, \\ H_e(S_n, x) &= \frac{n(n-1)}{2}x. \end{aligned}$$

Proposition 5 *For the wheel W_n with $n+1$ vertices, $n \geq 3$, it holds*

$$H(W_n, x) = 2nx + \frac{n(n-3)}{2}x^2,$$
$$Sc(W_n, x) = n(n+9)x + 3n(n-3)x^2,$$
$$Gut(W_n, x) = 3n(n+3)x + \frac{9n(n-3)}{2}x^2,$$
$$H_e(W_n, x) = \frac{n(n+5)}{2}x + n(n-1)x^2 + \frac{n(n-5)}{2}x^3.$$

Proposition 6 *For the path P_n with n vertices, $n \geq 3$, it holds*

$$H(P_n, x) = \sum_{i=1}^{n-1}(n-i)x^i,$$
$$Sc(P_n, x) = \sum_{i=1}^{n-2}(4n-2-4i)x^i + 2x^{n-1},$$
$$Gut(P_n, x) = \sum_{i=1}^{n-2}4(n-1-i)x^i + x^{n-1},$$
$$H_e(P_n, x) = \sum_{i=1}^{n-2}(n-1-i)x^i.$$

4 Roots of modified degree-distance-based polynomials

In this section, we investigate some newly defined polynomials. In particular, we introduce the following modified polynomials of a connected graph G with at least two vertices:

$$H^*(G, x) = 1 - H(G, x),$$
$$Sc^*(G, x) = 1 - Sc(G, x),$$
$$Gut^*(G, x) = 1 - Gut(G, x),$$
$$H_e^*(G, x) = 1 - H_e(G, x).$$

The motivation for studying these polynomials comes from a result used in Dehmer et al. (2020a), see also Brezovnik et al. (2023).

Lemma 7 (Brezovnik et al. 2023; Dehmer et al. 2020a) *Let $Q(x) = q_1x + q_2x^2 + \cdots + q_nx^n$ be a polynomial, $n \in \mathbb{N}$, $q_i \in [0, \infty)$ for all $i \in \{1, \ldots, n\}$, and $q_1 + q_2 + \cdots + q_n \geq 1$. Then the polynomial $Q^*(x) = 1 - Q(x)$ has a unique positive root δ such that $\delta \in (0, 1]$. Moreover, $\delta = 1$ if and only if $q_1 + q_2 + \cdots + q_n = 1$.*

Definition 8 Let $Q(x) = q_1x + q_2x^2 + \cdots + q_nx^n$ be a polynomial, $n \in \mathbb{N}$, $q_i \in [0, \infty)$ for all $i \in \{1, \ldots, n\}$, and $q_1 + q_2 + \cdots + q_n \geq 1$. The unique positive root of the polynomial $Q^*(x) = 1 - Q(x)$ will be denoted as $\delta(Q^*(x))$.

Obviously, if a connected graph has at least two vertices, then the polynomials H, Sc, and Gut can be written as $q_1x + q_2x^2 + \cdots + q_nx^n$, where $n \in \mathbb{N}$, $q_i \in [0, \infty)$ for all $i \in \{1, \ldots, n\}$, and $q_1 + q_2 + \cdots + q_n \geq 1$. However, for the edge-Hosoya polynomial H_e we consider only connected graphs with at least three vertices, since otherwise $H_e(G, x) = 0$.

According to Lemma 7, each polynomial $Q^* \in \{H^*, H_e^*, Sc^*, Gut^*\}$ has a unique positive root, which always lies within the interval (0, 1]. This positive root serves as a topological index, referred to as a *root-index* (Brezovnik et al. 2023). In the rest of the section, we focus on some theoretical results regarding the obtained new root-indices of a graph G: the *Wiener root-index* $\delta(H^*(G, x))$, the *edge-Wiener root-index* $\delta(H_e^*(G, x))$, the *Schultz root-index* $\delta(Sc^*(G, x))$, and the *Gutman root-index* $\delta(Gut^*(G, x))$.

The next proposition follows by Lemma 7. More precisely, from the second part of the mentioned lemma it follows that the unique positive root of the modified polynomial equals one if and only if the sum of the coefficients of the original polynomial equals one.

Proposition 9 *Suppose G is a connected graph with at least one edge. If $Q^* = H^*$ or $Q^* = Gut^*$, then $\delta(Q^*(G, x)) = 1$ if and only if G is isomorphic to P_2. Moreover, $\delta(Sc^*(G, x)) < 1$. Furthermore, if G is a connected graph with at least two edges, then $\delta(H_e^*(G, x)) = 1$ if and only if G is isomorphic to P_3.*

Proof Obviously, $\sum_{k\geq 1} d_k(G) = 1$ if and only if G has only one pair of vertices, which is further equivalent to G being isomorphic to P_2. Analogous reasoning gives us the same conclusion for $\sum_{k\geq 1} g_k(G)$. On the other hand, since $s_1(G) \geq 2$, we have $\sum_{k\geq 1} s_k(G) > 1$, which implies $\delta(Sc^*(G, x)) < 1$. Finally, $\sum_{k\geq 1} d_k^e(G) = 1$ implies $d_1^e = 1$, which is true only if G has exactly two edges, so it should be isomorphic to P_3. Consequently, the stated proposition follows by Lemma 7. □

4.1 Lower bounds for root-indices

In what follows, we establish lower bounds for all investigated root-indices. Note that analogous results were obtained for some other root-indices (Brezovnik et al. 2023; Tratnik and Žigert Pleteršek 2024).

Theorem 10 *Let G be a connected graph with at least three vertices. Then*

$$\delta(H^*(G, x)) > \frac{1}{MH(G) + 1}, \quad \delta(Sc^*(G, x)) > \frac{1}{MS(G) + 1},$$
$$\delta(Gut^*(G, x)) > \frac{1}{MG(G) + 1}, \quad \delta(H_e^*(G, x)) > \frac{1}{MH_e(G) + 1}.$$

Proof The proof is analogous for all polynomials, so we consider only $\delta(H^*(G, x))$. Let $\delta = \delta(H^*(G, x))$. Obviously, the result holds trivially if $\delta = 1$, so in the following suppose that $\delta < 1$. We consider

$$H(G, \delta) = \sum_{k\geq 1} d_k(G)\delta^k,$$

where $d_k(G)$ is the number of pairs of vertices at distance k. We start with

$$H(G, \delta) = \sum_{k\geq 1} d_k(G)\delta^k < \sum_{k\geq 1} MH(G)\delta^k = MH(G) \sum_{k=1}^{\infty} \delta^k = MH(G)\frac{\delta}{1-\delta}.$$

Consequently, it holds

$$\sum_{k\geq 1} d_k(G)\delta^k < MH(G)\frac{\delta}{1-\delta}. \tag{1}$$

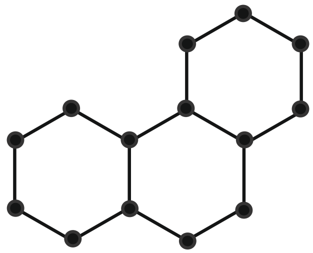

Fig. 1 Chemical graph G of phenanthrene

However, it is clear that

$$H^*(G, \delta) = 0,$$

so from $H^*(G, \delta) = 1 - H(G, \delta)$ we also get

$$H(G, \delta) = \sum_{k \geq 1} d_k(G)\delta^k = 1. \tag{2}$$

Finally, Eqs. (1) and (2) imply

$$1 < MH(G)\frac{\delta}{1-\delta},$$

which gives

$$\delta(H^*(G, x)) > \frac{1}{MH(G) + 1}.$$

□

For demonstration, we will compute the polynomials, root-indices, and lower bounds of a chemical graph G from Fig. 1.
The corresponding polynomials of G are

$$\begin{aligned} H(G, x) &= x^7 + 4x^6 + 10x^5 + 16x^4 + 22x^3 + 22x^2 + 16x, \\ H_e(G, x) &= 4x^6 + 10x^5 + 20x^4 + 33x^3 + 31x^2 + 22x, \\ Sc(G, x) &= 4x^7 + 16x^6 + 42x^5 + 70x^4 + 102x^3 + 106x^2 + 76x, \\ Gut(G, x) &= 4x^7 + 16x^6 + 44x^5 + 76x^4 + 117x^3 + 126x^2 + 91x. \end{aligned}$$

Consequently, we numerically obtain the root-indices of G:

$$\begin{aligned} \delta(H^*(G, x)) &\doteq 0.05765, \quad \delta(H_e^*(G, x)) \doteq 0.04276, \\ \delta(Sc^*(G, x)) &\doteq 0.01292, \quad \delta(Gut^*(G, x)) \doteq 0.01082. \end{aligned}$$

However, from the polynomials follows that

$$MH(G) = 22, \quad MH_e(G) = 33, \quad MS(G) = 106, \quad MG(G) = 126.$$

Hence, by Theorem 10 we get

$$\delta(H^*(G, x)) > \frac{1}{23} \doteq 0.04348, \quad \delta(H_e^*(G, x)) > \frac{1}{34} \doteq 0.02941,$$

$$\delta(Sc^*(G,x)) > \frac{1}{107} \doteq 0.00935, \quad \delta(Gut^*(G,x)) > \frac{1}{127} \doteq 0.00787.$$

We also notice that the lower bounds from Theorem 10 give good approximations for the root-indices of graph G.

4.2 Convergence of sequences of root-indices

In this subsection, we focus on the sequences of root-indices. To show their behavior for graphs with large order, we firstly prove the following theorem.

Theorem 11 *For any $n \geq 1$ let $Q_n(x) = q_{n,1}x + q_{n,2}x^2 + \cdots + q_{n,m_n}x^{m_n}$ be a polynomial such that $q_{n,i} \in [0,\infty)$ for all $i \in \{1,\ldots,m_n\}$ and $q_{n,1} + q_{n,2} + \cdots + q_{n,m_n} \geq 1$. Moreover, suppose that there exists a constant $k \geq 1$ and a function $f : \mathbb{N} \to \mathbb{R}$ such that*

$$\lim_{n\to\infty} f(n) = \infty$$

and for every $n \geq 1$ it holds $q_{n,k} = f(n)$. If $c_n = \delta(Q_n^*(x))$ for all $n \geq 1$, then the sequence (c_n) converges to 0:

$$\lim_{n\to\infty} c_n = 0.$$

Proof Obviously, for any $n \geq 1$ it holds

$$Q^*(c_n) = 1 - Q_n(c_n) = 0$$

and therefore

$$Q_n(c_n) = q_{n,1}c_n + q_{n,2}c_n^2 + \cdots + q_{n,m_n}c_n^{m_n} = 1.$$

Since the polynomial $Q_n(x)$ satisfies the conditions of Lemma 7 it follows that

$$0 \leq q_{n,k}c_n^k = f(n)c_n^k \leq 1$$

for all $n \geq 1$. Consequently, there exists $n_0 \geq 1$ such that for any $n \geq n_0$ it holds

$$0 \leq c_n^k \leq \frac{1}{f(n)} \quad \Longrightarrow \quad 0 \leq c_n \leq \frac{1}{\sqrt[k]{f(n)}}.$$

Since

$$\lim_{n\to\infty} \frac{1}{\sqrt[k]{f(n)}} = 0,$$

we have proved that the sequence (c_n) converges to 0. □

The special case of the above theorem is obtained if coefficients before x^k for some $k \geq 1$ are determined by a polynomial.

Corollary 12 *For any $n \geq 1$ let $Q_n(x) = q_{n,1}x + q_{n,2}x^2 + \cdots + q_{n,m_n}x^{m_n}$ be a polynomial such that $q_{n,i} \in [0,\infty)$ for all $i \in \{1,\ldots,m_n\}$ and $q_{n,1} + q_{n,2} + \cdots + q_{n,m_n} \geq 1$. Moreover, suppose that there exists a constant $k \geq 1$ and a polynomial p with degree at least one such that for every $n \geq 1$ it holds $q_{n,k} = p(n)$. If $c_n = \delta(Q_n^*(x))$ for all $n \geq 1$, then the sequence (c_n) converges to 0.*

As an example, we consider some basic families of graphs.

Corollary 13 *Let* $Q \in \{H, Sc, Gut, H_e\}$ *be a polynomial and for any* $n \geq 3$ *let* $G_n \in \{K_n, C_n, S_n, W_n, P_n\}$. *Then we have*

$$\lim_{n\to\infty} \delta(Q^*(G_n, x)) = 0.$$

Proof The result follows directly from Corollary 12 and Propositions 1 to 6. □

By using Proposition 1 we can also obtain explicit formulas for three root-indices of complete graphs.

Proposition 14 *For the complete graph* K_n *on* n *vertices,* $n \geq 2$, *it follows*

$$\delta(H^*(K_n, x)) = \frac{2}{n(n-1)},$$
$$\delta(Sc^*(K_n, x)) = \frac{1}{n(n-1)^2},$$
$$\delta(Gut^*(K_n, x)) = \frac{2}{n(n-1)^3}.$$

It turns out that to show a sequence of root-indices converges to zero, it is sufficient to verify that the number of edges in the corresponding sequence of graphs tends to infinity.

Theorem 15 *For any* $n \geq 1$ *let* G_n *be a connected graph with at least three vertices. Moreover, let* $Q \in \{H, Sc, Gut, H_e\}$ *be a polynomial. If*

$$\lim_{n\to\infty} |E(G_n)| = \infty,$$

then

$$\lim_{n\to\infty} \delta(Q^*(G_n, x)) = 0.$$

Proof Let $q_{n,1}$ be the coefficient in front of x of the polynomial $Q(x)$. If $Q = H$ is the Hosoya polynomial, then $q_{n,1} = |E(G_n)|$ for any $n \geq 1$. Since

$$\lim_{n\to\infty} |E(G_n)| = \infty,$$

the result follows by Theorem 11.

Next, let $Q = Sc$ be the Schultz polynomial. Then for any $n \geq 1$,

$$\begin{aligned} q_{n,1} &= \sum_{\substack{\{a,b\}\subseteq V(G_n) \\ d(a,b)=1}} (\deg(a) + \deg(b)) \\ &= \sum_{ab\in E(G_n)} (\deg(a) + \deg(b)) \geq \sum_{ab\in E(G_n)} 1 = |E(G_n)|. \end{aligned}$$

Since

$$\lim_{n\to\infty} |E(G_n)| = \infty,$$

it follows

$$\lim_{n\to\infty} q_{n,1} = \infty$$

and by Theorem 11 also

$$\lim_{n\to\infty} \delta(Q^*(G_n, x)) = 0.$$

Moreover, let $Q = Gut$ be the Gutman polynomial. Then for any $n \geq 1$,

$$q_{n,1} = \sum_{\substack{\{a,b\}\subseteq V(G_n)\\ d(a,b)=1}} \deg(a)\deg(b)$$
$$= \sum_{ab\in E(G_n)} \deg(a)\deg(b) \geq \sum_{ab\in E(G_n)} 1 = |E(G_n)|.$$

Since

$$\lim_{n\to\infty} |E(G_n)| = \infty,$$

it follows

$$\lim_{n\to\infty} q_{n,1} = \infty$$

and the result is obtained by Theorem 11.

Finally, let $Q = H_e$ be the edge-Hosoya polynomial. Obviously, for any $n \geq 1$,

$$q_{n,1} = |E(L(G_n))|.$$

Choose any $n \geq 1$. Let $E(G_n) = \{e_1, e_2, \ldots, e_m\}$ be the set of edges of the graph G_n, where $m = |E(G_n)|$. For any edge e_i from $E(G_n)$, let e_i^* be an arbitrarily chosen edge of $L(G_n)$ such that e_i is an end vertex of e_i^*. Then, let

$$R = \{e_1^*, e_2^*, \ldots, e_m^*\}.$$

Note that for any $i \in \{1, \ldots, m\}$, there exists at most one $j \in \{1, \ldots, m\} \setminus \{i\}$, such that $e_i^* = e_j^*$. Denote by $r = |R|$ the number of distinct elements of R. It follows that

$$r \geq \frac{m}{2},$$

which implies

$$q_{n,1} = |E(L(G_n))| \geq r \geq \frac{m}{2} = \frac{|E(G_n)|}{2}.$$

By similar arguments as before we obtain

$$\lim_{n\to\infty} q_{n,1} = \infty,$$

so the result follows. □

Remark 16 Let G be a connected graph with at least two vertices and let $q_{n,1}$ be the coefficient in front of x of the Schultz polynomial $Sc(G, x)$. From the proof of the previous theorem we observe that

$$q_{n,1} = \sum_{ab\in E(G_n)} (\deg(a) + \deg(b)) = M_1(G),$$

where $M_1(G)$ is the first Zagreb index of G (Gutman and Trinajstić 1972).

Similarly, if $q_{n,1}$ is the coefficient in front of x of the Gutman polynomial $Gut(G, x)$, then

$$q_{n,1} = \sum_{ab\in E(G_n)} \deg(a)\deg(b) = M_2(G),$$

where $M_2(G)$ is the second Zagreb index of G (Gutman and Trinajstić 1972).

Since the number of edges of a connected graph G with $|V(G)|$ vertices is at least $|V(G)|-1$, we immediately obtain the next corollary.

Corollary 17 *For any $n \geq 1$ let G_n be a connected graph with at least three vertices. Moreover, let $Q \in \{H, Sc, Gut, H_e\}$ be a polynomial. If*

$$\lim_{n\to\infty} |V(G_n)| = \infty,$$

then

$$\lim_{n\to\infty} \delta(Q^*(G_n, x)) = 0.$$

Note that for well-known families (sequences) of chemical graphs, for example linear benzenoid chains, fibonacenes, phenylene chains, circumcoronene series, etc., the number of vertices is strictly increasing, so by Corollary 17, the sequences of investigated root-indices converge to zero.

5 Numerical results

Various numerical results related to the Wiener, Gutman, Schultz, and edge-Wiener root-indices are presented and evaluated in this section. All computations and graphical representations for this section were carried out using the SageMath (2025) mathematical software system, accessed through the CoCalc (2025) online platform. With N_j and T_j we denote the families of all connected graphs and all trees on j vertices, respectively.

5.1 Discrimination power

Firstly, we consider the discrimination power of root-indices. In particular, we investigate the discrimination (also called sensitivity) which was introduced in Konstantinova (1996). Let $\mathcal{F}$ be a finite family of graphs that are pairwise non-isomorphic. Moreover, let I be a topological index and $\mathcal{C}$ the set of all graphs G from $\mathcal{F}$ for which there exists a graph $H \in \mathcal{F}$ such that G and H are not isomorphic but $I(G) = I(H)$. With other words, $\mathcal{C}$ is the set of graphs that cannot be distinguished by topological index I. In addition, let $ND = |\mathcal{C}|$. The *discrimination* $Dis(I)$ of a topological index I is defined as

$$Dis(I) = \frac{|\mathcal{F}| - ND}{|\mathcal{F}|}.$$

For the families N_j, where $j \in \{5, 6, 7, 8\}$, and T_j, where $j \in \{8, \ldots, 16\}$, we have computed ND and Dis for all four investigated root-indices, see Table 1.

We can conclude that the Gutman root-index has the best discrimination power among all connected graphs. For example, this index can completely discriminate connected graphs on 5 vertices and it can discriminate more than 87% of connected graphs on 6 vertices, while on the other hand the Wiener root-index can discriminate only approximately 16% of them. As it turns out, the worst discrimination ability in all the mentioned families of connected graphs is obtained for the Wiener root-index. However, in the families of trees all four root-indices have almost the same discrimination power, which is very high. For example, they can distinguish all trees on 8 vertices and almost 80% of trees on 16 vertices.

To validate the introduction of new structural descriptors, we compare their performance with that of existing similar descriptors. We calculate the discrimination for all four standard

Table 1 Discrimination for considered root-indices in different families of graphs

Family	No. of graphs	$\delta(H^*)$		$\delta(Gut^*)$		$\delta(Sc^*)$		$\delta(H_e^*)$	
		ND	Dis	ND	Dis	ND	Dis	ND	Dis
Families of connected graphs									
N_5	21	14	0.3333	0	1.0000	4	0.8095	4	0.8095
N_6	112	94	0.1607	14	0.8750	51	0.5446	62	0.4464
N_7	853	811	0.0492	279	0.6729	588	0.3107	694	0.1864
N_8	11,117	11,014	0.0093	7010	0.3694	9823	0.1164	10,523	0.0534
Families of trees									
T_8	23	0	1.0000	0	1.0000	0	1.0000	0	1.0000
T_9	47	4	0.9149	4	0.9149	4	0.9149	4	0.9149
T_{10}	106	4	0.9623	4	0.9623	4	0.9623	4	0.9623
T_{11}	235	39	0.8340	39	0.8340	39	0.8340	39	0.8340
T_{12}	551	58	0.8947	58	0.8947	58	0.8947	58	0.8947
T_{13}	1301	214	0.8355	214	0.8355	214	0.8355	214	0.8355
T_{14}	3159	498	0.8424	498	0.8424	498	0.8424	498	0.8424
T_{15}	7741	1609	0.7921	1609	0.7921	1611	0.7919	1609	0.7921
T_{16}	19,320	3873	0.7995	3877	0.7993	3889	0.7987	3873	0.7995

Table 2 Discrimination for considered standard indices in different families of graphs

Family	No. of graphs	W		Gut		Sc		W_e	
		ND	Dis	ND	Dis	ND	Dis	ND	Dis
Families of connected graphs									
N_5	21	16	0.2381	2	0.9048	8	0.6190	7	0.6667
N_6	112	108	0.0357	41	0.6339	96	0.1429	91	0.1875
N_7	853	847	0.0070	715	0.1618	826	0.0317	829	0.0281
N_8	11,117	11,110	0.0006	10,998	0.0107	11,099	0.0016	11,085	0.0029
Families of trees									
T_8	23	6	0.7391	6	0.7391	6	0.7391	6	0.7391
T_9	47	39	0.1702	39	0.1702	39	0.1702	39	0.1702
T_{10}	106	83	0.2170	83	0.2170	83	0.2170	83	0.2170
T_{11}	235	221	0.0596	221	0.0596	221	0.0596	221	0.0596
T_{12}	551	528	0.0417	528	0.0417	528	0.0417	528	0.0417
T_{13}	1301	1286	0.0115	1286	0.0115	1286	0.0115	1286	0.0115
T_{14}	3159	3131	0.0089	3131	0.0089	3131	0.0089	3131	0.0089
T_{15}	7741	7724	0.0022	7724	0.0022	7724	0.0022	7724	0.0022
T_{16}	19,320	19,289	0.0016	19,289	0.0016	19,289	0.0016	19,289	0.0016

versions of the corresponding indices: the Wiener index, the Gutman index, the Schultz index, and the edge-Wiener index, see Table 2.

The results demonstrate that the considered root-indices outperform the standard versions of indices in terms of discrimination power, with this difference being particularly noticeable in families of trees. For instance, the Gutman root-index can discriminate more than 67%

Table 3 Correlation coefficients between root-indices in graph families T_{15} and N_8

Graph family	Root-index	$\delta(Gut^*)$	$\delta(Sc^*)$	$\delta(H_e^*)$
T_{15}	$\delta(H^*)$	0.9324	0.9872	0.9681
	$\delta(Gut^*)$		0.9479	0.9617
	$\delta(Sc^*)$			0.9945
N_8	$\delta(H^*)$	0.9440	0.9784	0.9591
	$\delta(Gut^*)$		0.9873	0.9953
	$\delta(Sc^*)$			0.9959

Table 4 Correlation coefficients between standard indices in graph families T_{15} and N_8

Graph family	Index	Gut	Sc	W_e
T_{15}	W	1.0000	1.0000	1.0000
	Gut		1.0000	1.0000
	Sc			1.0000
N_8	W	−0.8598	−0.7646	−0.8518
	Gut		0.9614	0.9933
	Sc			0.9422

of all connected graphs with 7 vertices, whereas the Gutman index can distinguish less than 17% of these graphs. Remarkably, the mentioned root-index can distinguish almost 80% of trees with 16 vertices, whereas the corresponding index demonstrates a significantly lower discrimination rate of less than 0.2%.

5.2 Correlations

We further consider correlations between different pairs of root-indices. Two sets of samples are examined: all 11,117 connected graphs on 8 vertices and the complete collection of 7741 trees on 15 vertices. The Pearson correlation coefficients are collected in Table 3. It can be observed that the correlations are very strong, since the Pearson correlation coefficient in all cases is greater than 0.93.

We also compared the corresponding standard topological indices and the correlation coefficients are gathered in Table 4. We notice that for graph family T_{15}, there is a linear relation between any pair of topological indices. This is due to the facts that if T is a tree on n vertices, then $Gut(T) = 4W(T) - 2n^2 + 3n - 1$ (Gutman 1994), $Sc(T) = 4W(T) - n^2 + n$ (Klein et al. 1992; Gutman 1994), and $W_e(T) = W(T) - \frac{n^2-n}{2}$ (Buckley 1981). On the other hand, in the family N_8 we do not have linear relations, although the correlations are still quite good. It is also interesting that in N_8, the Wiener index negatively correlates with other standard topological indices.

In addition, we computed correlations between original indices and root-indices in two families of graphs, see Table 5. All the correlations are quite strong, but the best one is obtained between the Wiener index and the Wiener root-index in the family of all connected graphs on 8 vertices. Moreover, it is interesting that in the same family of graphs, all pairs of indices that do not include the Wiener index are negatively correlated.

Finally, we visualize the result from Tables 3, 4, and 5, see Fig. 2 for the family of trees on 15 vertices and Fig. 3 for the family of all connected graphs on 8 vertices. In the two

Table 5 Correlation coefficients between root-indices and standard indices in graph families T_{15} and N_8

Graph family	Index	W	Gut	Sc	W_e
T_{15}	$\delta(H^*)$	0.8046	0.8046	0.8046	0.8046
	$\delta(Gut^*)$	0.9300	0.9300	0.9300	0.9300
	$\delta(Sc^*)$	0.8153	0.8153	0.8153	0.8153
	$\delta(H_e^*)$	0.8394	0.8394	0.8394	0.8394
N_8	$\delta(H^*)$	0.9579	−0.9284	−0.8990	−0.9178
	$\delta(Gut^*)$	0.9050	−0.7781	−0.7707	−0.7673
	$\delta(Sc^*)$	0.9401	−0.8485	−0.8248	−0.8419
	$\delta(H_e^*)$	0.9292	−0.8071	−0.7835	−0.7996

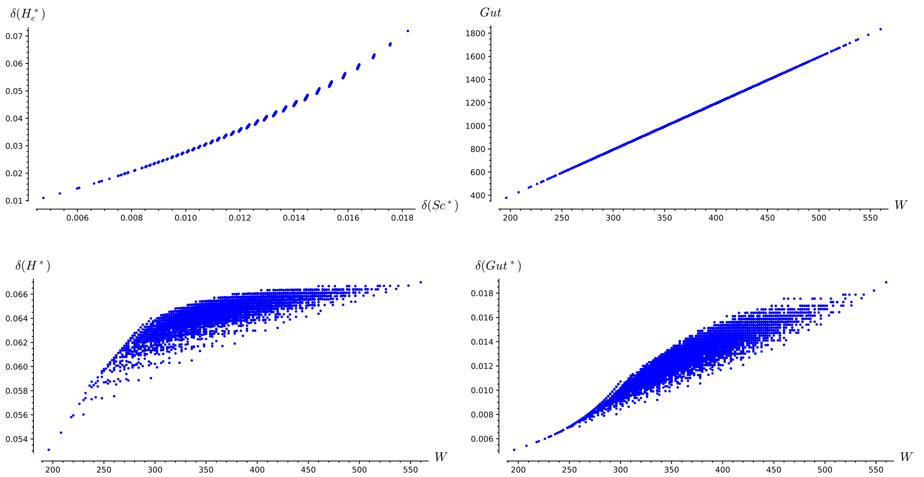

Fig. 2 Scatter plots for some pairs of considered topological (root-)indices on graph family T_{15}

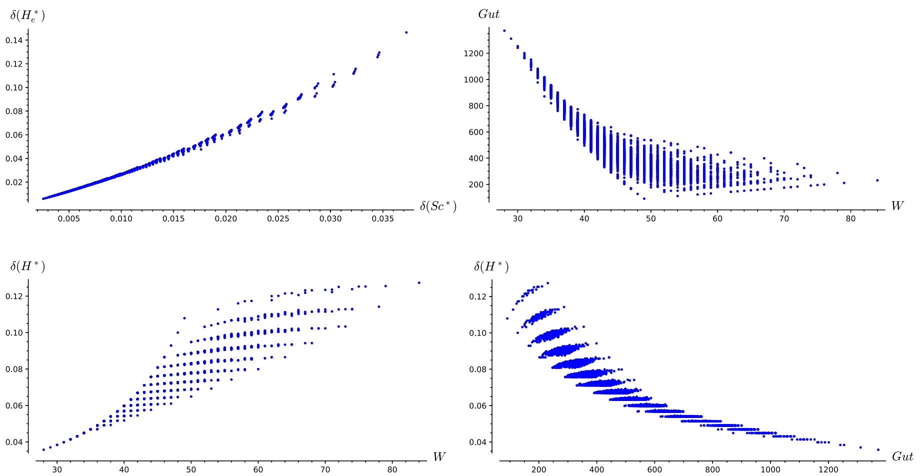

Fig. 3 Scatter plots for some pairs of considered topological (root-)indices on graph family N_8

scatter plots at the bottom of Fig. 2, we can clearly see that on trees the root-indices have better discrimination power than the standard indices. On the other hand, this is not true for the case of the Wiener index and the Wiener root-index (see the scatter plot in the lower left of Fig. 3), which coincides with the results from Tables 1 and 2.

5.3 Structure sensitivity and abruptness

Finally, we investigate some quantities which measure how a gradual change of a graph results on the topological index. We need several additional concepts.

Let $\mathcal{F}$ be a family of connected graphs and let $G \in \mathcal{F}$. Furthermore, let $\mathcal{S}(G)$ denote the collection of all pairwise non-isomorphic graphs that can be derived from G by the addition of precisely one edge. Consequently, the Graph Edit Distance (GED) between G and any graph within $\mathcal{S}(G)$ is equal to one (Gao et al. 2010; Sanfeliu and Fu 1983).

The *structure sensitivity* of a topological index I for the graph G, $SS_G^1(I)$, is defined in the following way (Furtula et al. 2013; Rakić and Furtula 2019):

$$SS_G^1(I) = \frac{1}{|\mathcal{S}(G)|} \sum_{G' \in \mathcal{S}(G)} \left| \frac{I(G) - I(G')}{I(G)} \right|.$$

Moreover, the *abruptness* of I for the graph G, $Abr_G^1(I)$, is calculated as

$$Abr_G^1(I) = \max_{G' \in \mathcal{S}(G)} \left| \frac{I(G) - I(G')}{I(G)} \right|.$$

Furthermore, in Rakić and Furtula (2019) the authors proposed different versions of structure sensitivity, $SS_G^2(I)$, and abruptness, $Abr_G^2(I)$, of a graph G for a topological index I:

$$SS_G^2(I) = \sqrt{\frac{1}{|\mathcal{S}(G)|} \sum_{G' \in \mathcal{S}(G)} (I(G) - I(G'))^2},$$

$$Abr_G^2(I) = \max_{G' \in \mathcal{S}(G)} \left| I(G) - I(G') \right|.$$

The structure sensitivity and abruptness of a topological index I on a family of graphs $\mathcal{F}$ is defined as the average over all elements of $\mathcal{F}$. So, for $i \in \{1, 2\}$, we have

$$SS^i(I) = \frac{1}{|\mathcal{F}|} \sum_{G \in \mathcal{F}} SS_G^i(I),$$

$$Abr^i(I) = \frac{1}{|\mathcal{F}|} \sum_{G \in \mathcal{F}} Abr_G^i(I).$$

It is preferred for a topological index to have the structure sensitivity as large as possible and the abruptness as small as possible (Furtula et al. 2013). If a topological index fulfils this property, on the one hand it can distinguish well between similar graphs, but on the other hand there is not much difference between the changes in the topological index. Therefore, it seems reasonable to introduce a new measure SA^i, $i \in \{1, 2\}$, as

$$SA^i(I) = \frac{SS^i(I)}{Abr^i(I)}.$$

Table 6 Structure sensitivity and abruptness of root-indices for all trees on n vertices, where $n \in \{9, 10, 11, 12\}$

Root-index	Graph class	SS^1	Abr^1	SA^1	SS^2	Abr^2	SA^2
$\delta(H^*)$	T_9	0.0977	0.1161	0.8417	0.0106	0.0125	0.8471
	T_{10}	0.0902	0.1080	0.8352	0.0088	0.0104	0.8405
	T_{11}	0.0837	0.1010	0.8288	0.0074	0.0089	0.8339
	T_{12}	0.0779	0.0943	0.8264	0.0063	0.0076	0.8312
$\delta(Gut^*)$	T_9	0.2794	0.3853	0.7252	0.0074	0.0099	0.7416
	T_{10}	0.2567	0.3708	0.6922	0.0058	0.0082	0.7123
	T_{11}	0.2381	0.3591	0.6632	0.0048	0.0069	0.6857
	T_{12}	0.2218	0.3470	0.6391	0.0040	0.0060	0.6637
$\delta(Sc^*)$	T_9	0.1845	0.2622	0.7038	0.0049	0.0068	0.7287
	T_{10}	0.1696	0.2480	0.6839	0.0040	0.0056	0.7103
	T_{11}	0.1569	0.2362	0.6646	0.0033	0.0048	0.6917
	T_{12}	0.1459	0.2244	0.6501	0.0028	0.0040	0.6776
$\delta(H_e^*)$	T_9	0.2288	0.3373	0.6784	0.0212	0.0298	0.7120
	T_{10}	0.2111	0.3218	0.6560	0.0170	0.0246	0.6915
	T_{11}	0.1960	0.3088	0.6349	0.0140	0.0208	0.6711
	T_{12}	0.1828	0.2954	0.6187	0.0117	0.0178	0.6554

The new measure enables us to compare different topological indices, since it is desired for the quotient SA^i, $i \in \{1, 2\}$, to be as large as possible. The results for both versions of structure sensitivity, abruptness, and their quotient of root-indices for the class of trees with n vertices, $n \in \{9, 10, 11, 12\}$, are shown in Table 6.

The results show that the best index regarding SA^1 and SA^2 is the Wiener root-index. For example, for trees on 11 vertices we get $SA^1(\delta(H^*)) = 0.8288$, $SA^1(\delta(Gut^*)) = 0.6632$, $SA^1(\delta(Sc^*)) = 0.6646$, $SA^1(\delta(H_e^*)) = 0.6349$ and similarly $SA^2(\delta(H^*)) = 0.8339$, $SA^2(\delta(Gut^*)) = 0.6857$, $SA^2(\delta(Sc^*)) = 0.6917$, $SA^2(\delta(H_e^*)) = 0.6711$. We also observe that on trees both measures, SA^1 and SA^2, behave very similarly for all four indices. Therefore, it seems that if we want to evaluate the performance of different topological indices on trees, it does not matter with which version we work.

6 Summary and conclusion

We introduced and examined several novel root-indices of graphs, which can be used as quantitative graph measures. Initially, we presented analytical findings related to the roots of new modified graph polynomials. More precisely, several closed formulas and bounds were determined. An important contribution is also the set of results related to the convergence of sequences of root-indices.

In Sect. 5, we performed quantitative analysis and compared the results to original topological descriptors. The results indicate that the new descriptors have significantly enhanced discrimination power. Among connected graphs, the Gutman root-index shows the highest discrimination power. However, for tree families, all four root-indices exhibit almost identical, high discrimination power. Moreover, it can be observed that the correlations between different root-indices are very strong, in all cases greater than 0.93. Additionally, the correlations between root-indices and their original versions are also quite high, which means that the root-indices capture information similarly as other standard (existing) graph measures. On the other hand, it seems better to use root-indices since they have much higher discrimination power.

Regarding structure sensitivity and abruptness, which quantify how a gradual change of a graph results on the topological index, we introduced their quotient as a new measure in order to simplify the comparison of different topological indices. We found out that the best index regarding the mentioned new measure is the Wiener root-index.

As a future work, we would like to improve the stated bounds by finding novel estimations. We are convinced that these bounds can be generalized such that the presented bounds will result as special cases. Also, we want to prove more upper and lower bounds for these measures by considering similar or other graph polynomials and compare the results with the ones we have stated in this paper. Another idea is to prove so-called implicit bounds (Dehmer and Mowshowitz 2011). Finally, we would like to investigate chemical applications of various root-indices.

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Data availability All the computational results supporting the findings of this study are available within the paper.

Declarations

Conflict of interest The author declares that there is no conflict of interest.

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