MATCH
Communications in Mathematical and in Computer Chemistry

MATCH Commun. Math. Comput. Chem. 93 (2025) 247–263
ISSN: 0340–6253
doi: 10.46793/match.93-1.247F

Complementary Topological Indices

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(Received February 20, 2024)

Abstract

An edge of a graph can be geometrically represented by points (d_r, d_s) and (d_s, d_r) in a 2D coordinate system, where coordinates are, obviously, the degrees of the edge's end-vertices. Recently, using such a geometrical point of view of a graph edge, a couple of topological invariants were put forward. They have attracted considerable attention among chemical graph theorists. This paper introduces a novel approach for devising "geometrical" topological indices. Finally, special attention is focused on the complementary second Zagreb index as a representative of the introduced approach.

1 Introduction

Molecular descriptors are necessary tools for quantifying the structure of a molecule [19, 20]. There are many molecular descriptors, and they are grouped into several classes [2,20]. The class containing topological indices is probably the largest one [2, 4]. They are heavily employed in diverse chemical investigations [2–4, 19, 20]. This is one of the reasons for the immense interest in these indices and the steep multiplication of their number.

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Graph features used in the definition of a topological index determine its affiliation to one of the distinct classes of these descriptors. Thus, one can differentiate degree-based, distance-based, and eigenvalue-based topological indices, among others. The degree-based topological descriptors are one of the largest groups among topological indices. There are myriad degree-based topological indices.

The degree-based topological indices, defined using a "geometrical" approach, have attracted significant attention and are being extensively investigated. The first and most significant representative is certainly the Sombor index [6]. Despite its juvenility, several hundreds of research papers have been published (e.g. see [8, 15, 17] and references cited therein), where the Sombor index was treated from various aspects.

Searching for suitable degree-based topological indices has been an ongoing task. Recently, a novel approach was put forward for devising the "geometrical" degree-based topological indices. Thus, an elliptic Sombor index was introduced [8].

We present here a novel way of contemplating the concept of "geometrical" degree-based topological indices, where the *angle of an edge* and its complement are introduced. By applying this approach we come up with the definition of the earlier introduced *nano Zagreb index* [11], or the F-minus index [13], or the *first Sombor index* [10, 18]. We think these names are less adequate for this index and propose renaming it to the *complement second Zagreb index* (cM_2). We will use this name and notation in the rest of the text.

2 Method

An edge rs of a graph G with degrees d_r and d_s of end-vertices may be represented in a 2D coordinate system by the degree-point (d_r, d_s) and its dual-degree-point (d_s, d_r) [6]. These vectors intersect at the origin of the coordinate system and form an *angle of the edge*, α_{rs} (see Figure 1).

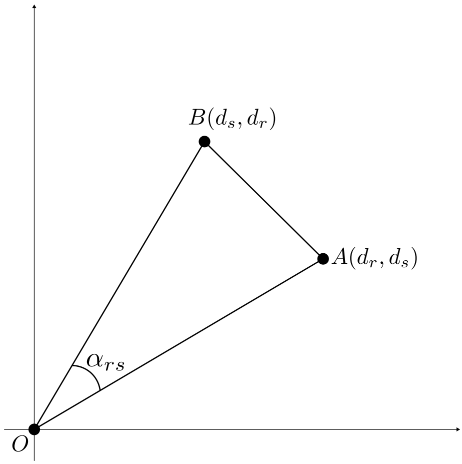


Figure 1. Degree-point, its dual-degree-point, and the edge angle.

The sine of the edge-angle can be calculated using the degrees of end-vertices of an edge.

Theorem 1. *Let rs be an edge of graph G. Let degrees of its end-vertices be d_r and d_s. It is assumed that $d_r \geqslant d_s$, without loss of generality. Then,*

$$\sin \alpha_{rs} = \frac{d_r^2 - d_s^2}{d_r^2 + d_s^2} \tag{1}$$

Proof. The area A_{AOB} is equal to

$$A_{AOB} = \frac{1}{2} \cdot \begin{vmatrix} d_r & d_s & 1 \\ d_s & d_r & 1 \\ 0 & 0 & 1 \end{vmatrix} = \frac{1}{2} \cdot \left(d_r^2 - d_s^2\right) \tag{2}$$

Knowing the lengths of vectors $|\overrightarrow{OA}| = |\overrightarrow{OB}| = \sqrt{d_r^2 + d_s^2}$, the area of the same triangle can be calculated as follows:

$$A_{AOB} = \frac{1}{2} \cdot |\overrightarrow{OA}| \cdot |\overrightarrow{OB}| \cdot \sin \alpha_{rs} = \frac{1}{2} \cdot \left(d_r^2 + d_s^2\right) \cdot \sin \alpha_{rs} \tag{3}$$

Combining Eqs. (2) and (3), the formula given in Eq. (1) is obtained. ∎

The sine of the complement of the edge-angle β_{rs} is given in the Theorem 2.

Theorem 2. *Assuming without loss of the generality that $d_r \geqslant d_s$, the sine of the complement angle β_{rs} of the edge-angle α_{rs} is*

$$\sin\beta_{rs} = \frac{(d_r + d_s)^2 - (d_r - d_s)^2}{(d_r + d_s)^2 + (d_r - d_s)^2} \tag{4}$$

Proof. It is well-known that

$$\sin\beta_{rs} = \sin(90^\circ - \alpha_{rs}) = \cos\alpha_{rs}\ .$$

The cosine of the edge-angle is calculated from its sine given in the Eq. (4)

$$\sin\beta_{rs} = \sqrt{1 - \sin^2\alpha_{rs}} = \frac{2d_r\, d_s}{d_r^2 + d_s^2}\ . \tag{5}$$

Equation (5) is rewritten as follows:

$$\sin\beta_{rs} = \frac{2 \cdot 2d_r\, d_s}{2d_r^2 + 2d_s^2} = \frac{(d_r^2 + 2d_r\, d_s + d_s^2) - (d_r^2 - 2d_r\, d_s + d_s^2)}{(d_r^2 + 2d_r\, d_s + d_s^2) + (d_r^2 - 2d_r\, d_s + d_s^2)}\ .$$

Thus, we obtain the sine of a complement of the edge-angle given in the Eq. 4. ■

By inspecting the Eq. (1) it is evident that the calculation of the sine of the edge-angle is feasible by knowing the edge coordinates, i.e. the degree-point A and dual-degree-point B, shown in Figure 1. Similarly, for the calculation of the complement of the edge-angle using the Eq. (4) the complementary edge coordinates $A'(d_r{+}d_s, d_r{-}d_s)$ and $B'(d_r{-}d_s, d_r{+}d_s)$ are needed, as it is shown in Figure 2. The point A' will be named as the *complementary degree-point*, and B' as the *complementary dual-degree-point*.

There are two ways of devising topological invariants from the complementary degree-point and its dual. The first would be similar to the original "geometric" degree-based topological indices by obtaining the length of vectors, the circumference, or the area of geometrical shapes related to these coordinate points. As an example, the length of the vector $|\overrightarrow{OA'}|$ is equal to $\sqrt{2\,d_r^2 + 2\,d_s^2}$. Summing this contribution over all edges we come up to the Sombor index multiplied by $\sqrt{2}$. So, it is interesting that we are obtaining the Sombor index summing contributions of lengths either $|\overrightarrow{OA}|$ or $|\overrightarrow{OA'}|$ over all edges. Further, by summing contributions of the area of the $\triangle OA'B'$ (see Figure 2) over all edges, we get $2 \cdot M_2(G)$. This may be seen as a geometrical interpretation of the second Zagreb index.

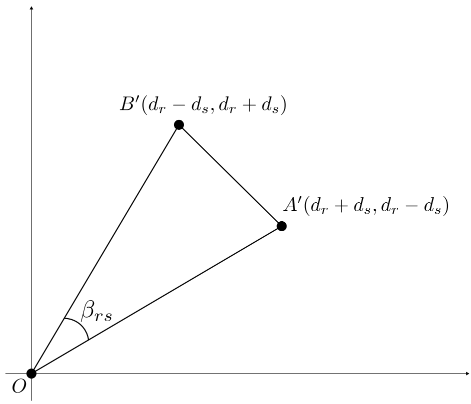


Figure 2. Complementary degree-point, its complementary dual-degree-point, and the complement of the edge angle.

The other way to construct the indices using complement degree points is by substituting end-vertex degrees d_r and d_s with $d_r + d_s$ and $d_r - d_s$ in the definitions of the existing degree-based topological indices. Using this approach we get a whole new group of degree topological descriptors that we named as *complementary topological indices*. In this way, the complementary indices of some well-known degree-based topological indices can be constructed, as shown in Table 1.

Table 1. Definitions of the complementary indices of some frequently used degree-based representatives. It is assumed that $d_r \geqslant d_s$.

Degree-based TI	**Complementary TI**
$M_1(G) = \sum_{rs}(d_r + d_s)$	$cM_1(G) = 2\sum_{rs} d_r$

Degree-based TI	**Complementary TI**
$M_2(G) = \sum_{rs} d_r \cdot d_s$	$cM_2(G) = \sum_{rs} (d_r^2 - d_s^2)$
$F(G) = \sum_{rs} (d_r^2 + d_s^2)$	$cF(G) = 2 \cdot F(G) = 2 \sum_{rs} (d_r^2 + d_s^2)$
$GA(G) = \sum\limits_{rs} \frac{2\sqrt{d_r \cdot d_s}}{d_r + d_s}$	$cGA(G) = \sum\limits_{rs} \frac{\sqrt{d_r^2 - d_s^2}}{d_r}$
$AZI(G) = \sum\limits_{rs} \left(\frac{d_r \cdot d_s}{d_r + d_s - 2} \right)^3$	$cAZI(G) = \frac{1}{8} \sum\limits_{rs} \left(\frac{d_r^2 - d_s^2}{d_r - 1} \right)^3$
$ISI(G) = \sum\limits_{rs} \frac{d_r \cdot d_s}{d_r + d_s}$	$cISI(G) = \frac{1}{2} \sum\limits_{rs} \frac{d_r^2 - d_s^2}{d_r}$
$H(G) = \sum\limits_{rs} \frac{2}{d_r + d_s}$	$cH(G) = \sum\limits_{rs} \frac{1}{d_r}$
$SCI(G) = \sum\limits_{rs} \frac{1}{\sqrt{d_r + d_s}}$	$cSCI(G) = \frac{1}{\sqrt{2}} \sum\limits_{rs} \frac{1}{\sqrt{d_r}}$
$HM(G) = \sum\limits_{rs} (d_r + d_s)^2$	$cHM(G) = 4 \sum\limits_{rs} d_r^2$

In Table 1 are given the definitions of the first and second Zagreb indices ($M_1(G)$ and $M_2(G)$), forgotten index (F), geometric–arithmetic index ($GA(G)$), augmented Zagreb index ($AZI(G)$), inverse sum indeg index ($ISI(G)$), harmonic index ($H(G)$), sum-connectivity index ($SCI(G)$), hyper-Zagreb index ($HM(G)$), and their complementary indices respectively.

However, it should be aware that the complementary counterparts of some well-known degree-based topological indices are ill-defined, and as such, they can be applied in some quite limited cases. In principle, the complementary indices of degree-based topological invariants with a product of degrees of end-vertices in the denominator belong to this group. The Randić index, atom-bond connectivity index, and symmetric division deg index are invariants with ill-defined complementary indices.

Since the complementary first Zagreb index fully neglects the influence of the end-vertex with a smaller value of the degree, which is physically unjustifiable, we have focused on the next simplest complementary index.

In the next section, the main features of the complementary second Zagreb index are going to be reviewed.

3 Complementary second Zagreb index

Replacing values of degrees of end-vertices of an edge in the formula for the calculation of the second Zagreb index by the coordinates of the points that form the complement of the edge-angle is obtained formula of the *complementary second Zagreb index* (see Section 2):

$$cM_2(G) = \sum_{rs \in E(G)} d_r^2 - d_s^2 \tag{6}$$

where $d_r \geqslant d_s \ \forall rs \in E(G)$.

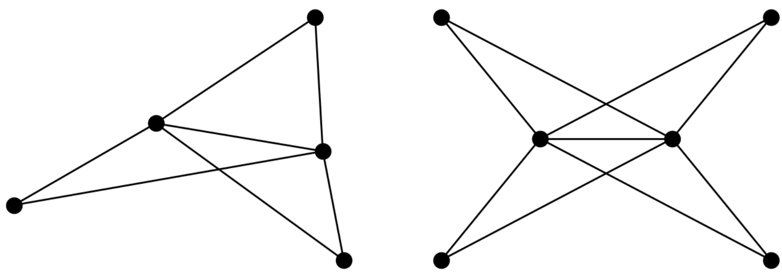
However, this index is not put forward here for the first time. It was introduced and reintroduced in several recent and unrelated papers, which resulted in several names for this index. According to our best knowledge, the first appearance of this index was in [11], where it was investigated for some products of graphs. There, this quantity was named the *nano Zagreb index.* This index was reintroduced in [13], where the author derived close formulas for this index in the case of some classes of dendrimers. He named it the *minus-F index.* Another appearance was found in [21], which authors called the *modified Albertson index.* In that paper, the authors considered this quantity as another measure of irregularity of graphs and derived a sharp lower bound in the case of trees and, also, characterized trees with minimal and maximal values of this quantity. To the best of our knowledge, the last reintroduction of this index was in [7], where the $1/2 \cdot |d_r^2 - d_s^2|$ is the area of the $\triangle OAB$ depicted in Figure 1. There, it was named the *first Sombor index.* In subsequent papers, this index was investigated for some supramolecular chains [10], and maximal trees and unicyclic graphs with some given parameters were determined in [14]. Additionally, in [14] the correlations of this index with some physicochemical properties of octanes and benzenoid hydrocarbons were displayed. This situation produces confusion in investigating this newly devised topological descriptor. So, according to the presented method of constructing this type of indices in the preceding section, we suggest that this index shall be called the *complementary second Zagreb index*.

In the rest of the article, we will fill some gaps in the elementary analysis of newly developed topological index.

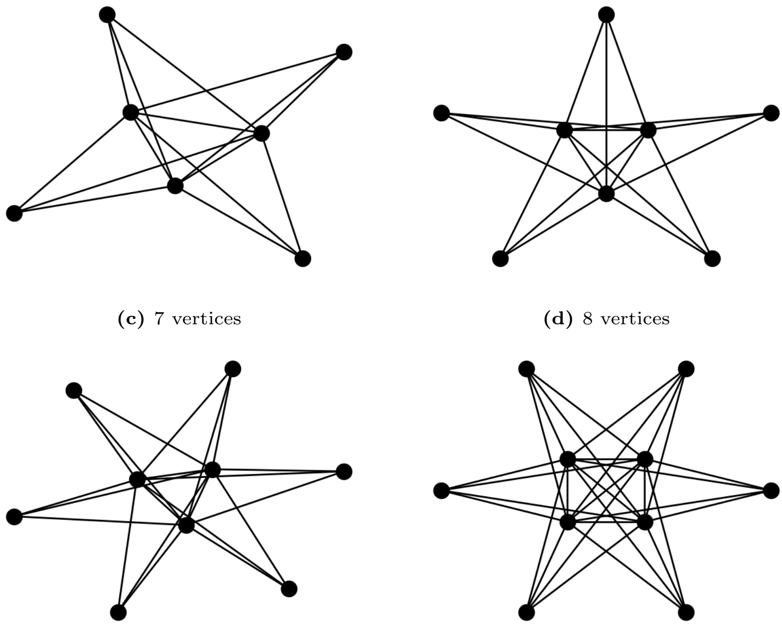
3.1 Extremal graphs

It was already mentioned that trees, having minimum and maximum $cM_2(G)$, were characterized in [21]. Also, the unicyclic graph with maximum complementary second Zagreb index was determined in [14].

Here, we will give a conjecture about the connected graph that maximizes $cM_2(G)$. Since the complementary second Zagreb index can be viewed as an irregularity measure, it is obvious that the regular graphs are one of the extrema among all connected graphs. In this particular case, the regular graphs have the minimum values of the $cM_2(G) = 0$. Finding the graph(s) with the maximum value of the $cM_2(G)$ is a much more complex problem. To get some feeling about the structure of a graph with the maximum value of the complementary second Zagreb index we performed a series of brute force searches over all connected graphs with 6 up to 10 vertices. Results are shown on the Figure 3.



(a) 5 vertices **(b)** 6 vertices



(c) 7 vertices (d) 8 vertices

(e) 9 vertices (f) 10 vertices

Figure 3. Connected graphs having maximum value of the $cM_2(G)$ index.

We failed to prove that the graphs depicted in Figure 3 maximize the complementary second Zagreb index, but their structure can be conjectured in the following manner:

Conjecture 1 (Structure of connected graph with the maximum $cM_2(G)$)**.** *Vertices in the connected graph with the maximal complementary second Zagreb index are partitioned into two groups. Let's label the number of vertices in the first group with k, which is always smaller than $\lceil n/2 \rceil$. These vertices form a k-complete subgraph. Each of the other $n-k$ vertices in this connected graph is connected to all vertices of the k-complete subgraph, but they are not mutually interconnected.*

Determining the order of the complete subgraph k, as a function of the number of vertices n of the connected graph that maximizes the value of the $cM_2(G)$, is far from being an easy task. We came up with a good linear correlation of k in terms of n, assuming that Conjecture 1 is valid. This correlation is given in Figure 4.

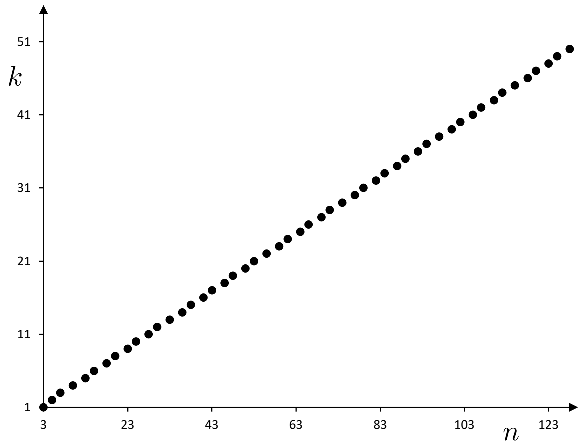


Figure 4. Correlation between the number of vertices of the complete subgraph versus the total number of vertices of a connected graph that maximizes the value of $cM_2(G)$.

The approximate linear equation that relates k and n is

$$k \approx \lfloor 0.391 \cdot n + 0.095 \rceil ,$$

where the correlation coefficient is equal to $R = 0.99995$. The obtained float number should be rounded to the closest integer.

3.2 Correlations with physicochemical properties

A large number of statistical data on linear regressions of the Sombor-like indices (including the complementary second Zagreb index) correlated with some common physicochemical properties of octanes and a set of benzenoid hydrocarbons were presented in [14]. There, it was demonstrated that $cM_2(G)$ model the heat of vaporization and, especially, the normalized heat of vaporization quite well.

Here, we give a comparison in modeling the physicochemical properties of octanes with the second Zagreb index versus the complementary second Zagreb index.

But, before presenting the main results of this comparative analysis, the correlation between second Zagreb and complementary second Zagreb indices was investigated. It was found that there is a fair correlation between these indices, but far from being good. This correlation for octanes is shown in the Figure 5.

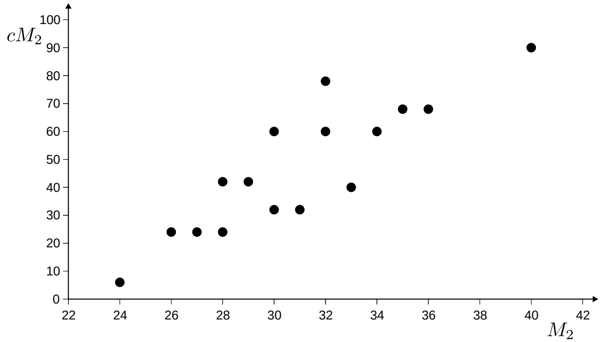


Figure 5. Correlation between second Zagreb index and complementary second Zagreb index. The correlation coefficient is 0.867.

Table 2 displays correlation coefficients of linear models of the several physicochemical properties of octanes with $M_2(G)$ and $cM_2(G)$.

Table 2. Correlation coefficients of the linear models of boiling point (BP), heat of formation (HFORM), standard heat of formation (DHFORM), entropy (S), heat of vaporization (HVAP), standard heat of vaporization (DHVAP), density (DENS), total surface area (TSA), acentric factor (AcentFac), octanol-water partition coefficient (LogP), and molar volume (MV) of octanes with second Zagreb index ($M_2(G)$) and complementary second Zagreb index ($cM_2(G)$), respectively.

	$M_2(G)$	$cM_2(G)$
BP	-0.5007	-0.7849
HFORM	-0.5421	-0.8234
DHFORM	0.4775	0.0500
S	-0.9417	-0.8899
HVAP	-0.7281	-0.9175

	$M_2(G)$	$cM_2(G)$
DHVAP	-0.8118	-0.9522
DENS	0.7303	0.4935
TSA	-0.5888	-0.2825
AcentFac	-0.9864	-0.9192
LogP	-0.1324	0.0638
MV	-0.7405	-0.4836

The linear models with $cM_2(G)$ of considerable quality are detected in the case of the heat of vaporization, standard heat of vaporization, and acentric factor. In all of these cases, the $cM_2(G)$ gives better linear models than the $M_2(G)$.

3.3 Degeneracy of complementary second Zagreb index

The degeneracy of a topological invariant informs us about its ability to discriminate among the isomeric graphs. A measure of degeneracy was proposed by Konstantinova in 1996 [12].

Using this way of measuring the degeneracy of topological descriptors, we assessed it for the $cM_2(G)$. Similar to the other integer-valued degree-based indices, the level of the degeneracy of the complementary second Zagreb index is extremely high, and, as shown in Table 3, the degeneracy rises with the number of vertices.

Table 3. Percentage of the degeneracy of $cM_2(G)$ in the case of all trees and chemical trees from 6 to 20 vertices.

n	# of trees	# of chemical trees
06	16.7%	20.0%
07	27.3%	33.3%
08	43.5%	50.0%

n	**# of trees**	**# of chemical trees**
09	57.4%	65.7%
10	70.8%	78.7%
11	80.0%	86.2%
12	87.3%	92.4%
13	92.3%	95.5%
14	95.5%	97.6%
15	97.5%	98.8%
16	98.7%	99.4%
17	99.3%	99.7%
18	99.7%	99.9%
19	99.8%	99.9%
20	99.9%	99.9%

According to these results for trees and chemical trees with 15 vertices and above, values of the $cM_2(G)$ of two randomly chosen trees are most likely the same. Such a behavior of a topological index is certainly not desirable.

3.4 Relations of complementary second Zagreb index with other topological indices

One of the features that tells us much about the behavior of a topological descriptor is its relations with other previously introduced indices. In Subsection 3.3, it was depicted the correlation between the considered complementary second Zagreb index and its counterpart, the second Zagreb index. This correlation is moderate, which implies that the $cM_2(G)$ encodes rather different structural details of graphs compared with the $M_2(G)$.

Since the $cM_2(G)$ is also the measure of irregularity in graphs, we analyzed its correlations with some known irregularity measures. In this investigation, we considered the Albertson index (Alb), the sigma index (σ), the degree variance (Var), the discrepancy ($Disc$), the Gini index (ζ), the normalized heterogeneity index (ρ), and the irregularity Sombor index (ISO). More on these indices can be found in [1,9]. Results will be illustrated with the correlation graph, given in Figure 6. There, the irregularity measures are represented by the vertices of the correlation graph. Two vertices are connected if the correlation coefficient obtained between two irregularity measures (represented by these vertices) is higher than 0.9. The edge is getting thicker with the higher value of the correlation coefficient.

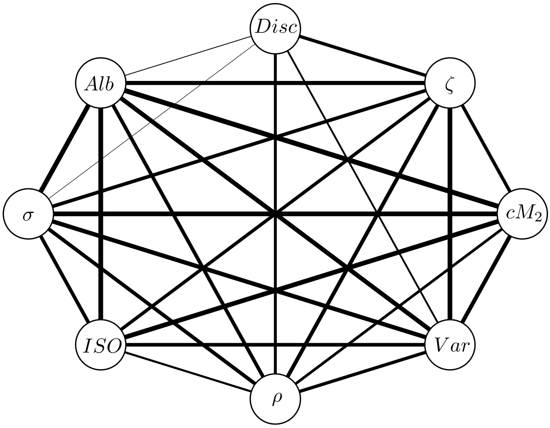


Figure 6. The correlation graph. Correlations coefficients needed for the constructing this graph are obtained on trees with 10 vertices.

Depicted graph in Figure 6 shows that the complementary second Zagreb index is highly correlated with the Albertson index ($R \approx 0.996$), the sigma index ($R \approx 0.991$), and the irregularity Sombor index ($R \approx 0.990$). Also, a noticeable correlation is detected with the degree variance ($R \approx 0.978$), the Gini index ($R \approx 0.964$), and the normalized heterogeneity index ($R \approx 0.952$). Therefore, the complementary second Zagreb index is expected to measure irregularity following all investigated irregularity measures, except the discrepancy index, defined based on the Randić index.

3.5 Sensitivity of complementary second Zagreb index

A gradual change in the structure of a graph should invoke a gradual change in the value of a topological index. Such a complex attribute of an index is being measured by two quantities that are named *structure sensitivity* (SS) and *abruptness* (Abr). There are two similar methods for calculating these quantities. Here, we mixed these two methods and took the best of them for assessing the structure sensitivity of $cM_2(G)$. Using a way for gathering similar graphs from [5], and a way for calculating the SS and the Abr from [16], we obtained results presented in Table 4 and Figure 7.

Table 4. The structure sensitivity and abruptness of the complementary second Zagreb index.

n	SS	Abr
6	0.267	0.360
7	0.173	0.248
8	0.112	0.176
9	0.078	0.130
10	0.055	0.097

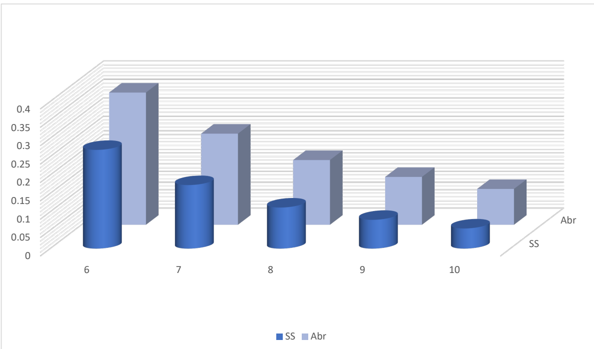


Figure 7. The structure sensitivity and abruptness of the complementary second Zagreb index.

The obtained results reveal similar behavior to the other integer-valued degree-based topological indices. In general, they have a low structure sensitivity that decreases as the number of vertices is increased. The abruptness follows the same line, but the ratio between structure sensitivity and abruptness increases with the number of vertices.

4 Conclusion

A novel geometric approach for devising degree-based topological indices is presented. We proposed to call this group of indices as *complementary topological indices*. The complementary second Zagreb index was thoroughly analyzed, and its upsides and downsides were displayed. We believe this approach will induce diverse investigations of this class of indices.

***Acknowledgment*:** The first author (B.F.) is partially financially supported by the Ministry of Science, Technological Development and Innovation of the Republic of Serbia through grant No. 451-03-65/2024-03/200122. The second author (M.S.O.) is financially supported by the Council of the Higher Education of Turkey.

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