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Research Paper

Bounds for Sombor index using topological and statistical indices

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Abstract. In this study, we find some bounds for the Sombor index of a graph G by some topological and statistical indices such as *arithmetic index*, *geometric index*, *arithmetic-geometric (AG) index*, *geometric-arithmetic (GA) index*, *symmetric division degree index (SDD(G))*, and some central and dispersion indices. The bounds can state estimated values and error intervals for the Somber index and show limits of accuracy. Error intervals are expressed as inequalities.

Keywords. Sombor index, topological indices, statistical indices, geometric-arithmetic index, arithmetic-geometric index.
Mathematics Subject Classification (2020): 05C09, 05C90.

1 Introduction

Topological indices are numerical parameters of graphs that are invariant under graph isomorphism and provide valuable insights into the structural properties of chemical compounds and their analysis. The Sombor index, introduced recently by Ivan Gutman, is one of these indices and has gained attention for its ability to obtain various structural features of graphs and predict the physicochemical properties of molecules. This index has been surveyed for some graphs by Aguilar, Das et al., Ghanbari and Alikhani, Kulli, Milovanović et al., and Mohammadi et al., in articles such as [1], [7], [11], [17], [20], and [21].

Despite the growing interest in the Sombor index, there is still much to explore, partic-

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ularly in terms of finding new bounds and relationships with other well-known topological indices. The goal of this paper is to provide a comprehensive set of bounds for the Sombor index using various mathematical techniques and statistical indices such as the AG index, GA index, variance, and standard deviation. In particular, these connections provide several benefits: Statistical indices allow for new bounds on the Sombor index and enhance the predictive power in both theoretical and applied contexts. Additionally, statistical indices help interpret the Sombor index in terms of independent properties of edges and how their distribution.

Some indices such as the arithmetic index and geometric index have been studied by Aldaz and Çelik in the articles such as [2], [3], the GA and AG indices by Cui et al., Chakrabarty, Das, Glaser, Rodin, Vujošević and et al. in the articles such as [6], [8], [9], [12], [23] and [26], and the SDD(G) index in the reference [27] by Vasilyev. Also, statistical studies on the Sombor index are done in th articles [1], [14] and [18]. In several papers, upper and lower bounds between the Sombor index, energy, and Laplacian energy of graphs are discussed, see for example [25] and [4].

In this article, we introduce these indices and establish new bounds that contribute to the ongoing research in this area.

Let $G = (V, E)$ ($|V(G)| = n$ and $|E(G)| = m$) be a graph. Then the Somber index is defined as follows

$$SO(G) = \sum_{uv \in E(G)} \sqrt{d^2(u) + d^2(v)}, \tag{1}$$

where $d(u)$ is the degree of vertex u in G.

2 Topological and Statistical Methods for Bounds of the Sombor index

In reference [7], using the elementary geometric method, a geometric view of the degrees of vertices using the Euclidean distance is introduced and could offer a different view of structural relationships in graphs even if the bounds aren't necessarily tighter. This approach could be useful in different contexts or types of graphs, such as random graphs. In this article, we use some definitions based on this article and prove some theorems.

The ordered pair $w = (d(u), d(v))$ is a point in the degree-coordinate (or d-coordinate) called the *degree-point* (or *d-point*) of the edge $uv \in E(G)$ where $d(u)$ denotes the degree of the vertex u and $d(v)$ the degree of the vertex v in the (2-dimensional) coordinate system. The point with coordinates $(d(v), d(u))$ is the *dual-degree* point (or *dd-point*) of the edge $uv \in E(G)$. The *degree-radius* (or *d-radius*) of the edge $uv \in E(G)$ is the Euclidean distance between $w = (d(u), d(v))$ and the origin of the coordinate system which is denoted by $z = |w| = \sqrt{d(u)^2 + d(v)^2}$. So,

$$\sqrt{2}z \geq d(u) + d(v). \tag{2}$$

Definition 2.1. *[3] The arithmetic mean for the nonnegative real numbers $x_1, x_2, \ldots, x_m$ is as*

$\mu = R_a = \frac{1}{m}\sum_{i=1}^{m} x_i$, for the geometric mean as $R_g = (\prod_{i=1}^{m} x_i)^{\frac{1}{m}} = \prod_{i=1}^{m} x_i^{\frac{1}{m}}$ and for the harmonic mean as $R_h = \frac{m}{\sum_{i=1}^{m}\frac{1}{x_i}}$.

Remark 2.2. *Note that inequality of arithmetic and geometric mean for the nonnegative real numbers $x_1, x_2, \ldots, x_m$ is as follows*

$$R_g = \prod_{i=1}^{m} x_i^{\frac{1}{m}} \leq \frac{1}{m}\sum_{i=1}^{m} x_i = R_a. \tag{3}$$

Equality holds whenever $x_1 = x_2 = \ldots = x_m$. Also, refering the reference [3], we could consider that for $i = 1, 2, \ldots, m$, if $\alpha = (\alpha_1, \alpha_2, \ldots, \alpha_m)$, $\alpha_i > 0$ and $\sum_{i=1}^{m}\alpha_i = 1$, then the general arithmetic-geometric inequality is $\prod_{i=1}^{m} x_i^{\alpha_i} \leq \sum_{i=1}^{m}\alpha_i x_i$. Also if apply the variable change $x_i = y_i^s$, then the general arithmetic-geometric inequality for $s > 0$ is as

$$\prod_{i=1}^{m} y_i^{\alpha_i} \leq (\sum_{i=1}^{m}\alpha_i y_i^s)^{\frac{1}{s}}, \tag{4}$$

and for $0 < s < 1$, Jensen's inequality tells us that

$$(\sum_{i=1}^{m}\alpha_i y_i^s)^{\frac{1}{s}} \leq \sum_{i=1}^{m}\alpha_i y_i, \tag{5}$$

since the function y^s is concave, and furthermore the inequality is strict unless $y_1 = y_2 = \ldots = y_m$ (this follows from the equality case in Jensen's inequality).

So, applying Inequalities (4) and (5) for $0 < s < 1$ we have

$$\prod_{i=1}^{m} y_i^{\alpha_i} \leq (\sum_{i=1}^{m}\alpha_i y_i^s)^{\frac{1}{s}} \leq \sum_{i=1}^{m}\alpha_i y_i.$$

Based on inequality (5), consider $\alpha_i = \frac{1}{m}$, $s = \frac{1}{2}$ and $y_i = d(u_i)^2 + d(v_i)^2 = z_i^2$, we have

$$SO(G) \leq \sqrt{F(G)m}, \tag{6}$$

in which $F(G) = \Sigma(d(u_i)^2 + d(v_i)^2)$. The index $F(G)$ is called the *forgotten index* and introduced in [10]. This relation is proved in [20] by another way.

Also, by appling inequality (3), if G is a graph with n vertices and m edges such that w_i for $i = 1, 2, \ldots, m$ be d-points related edges, then for the nonnegative numbers $z_1, z_2, \ldots, z_m$,

$$mR_g \leq SO(G).$$

Equality holds whenever $z_1 = z_2 = \ldots = z_m$. Now we intend to obtain upper and lower bounds for the Sombor index using the concept of variance in Theorems 2.4, 2.9, 2.11 and 2.14, which actually improve the aforementioned bounds.

In **[?]** discussed increasing linearly of the variance of topological indices which are sums of $f(d(u),d(v))$ for a function $f : \mathbb{N}^2 \rightarrow \mathbb{R}$ of a *random graph* with n vertices. As a result, we can explore the relationship between the Sombor index and statistical indices, such as the variance and geometric mean of degree points in a graph. By examining the variance of these degree points, we can evaluate the stability and variability of the Sombor index across various types of graphs, providing valuable insights into graph topology and structure.

Theorem 2.3. *[2, Th, 2.1] For $i = 1, 2, \ldots, m$, $x_i \geq 0$, and let $\alpha_i > 0$, $\beta_i > 0$ satisfy $\sum_{i=1}^{m} \alpha_i = \sum_{i=1}^{m} \beta_i = 1$. Writing $\alpha_{min} := min\{\alpha_1, \ldots, \alpha_m\}$, $\alpha_{max} = max\{\alpha_1, \ldots, \alpha_m\}$, and similarly for β_{min} and β_{max}, we have*

$$\min_{k=1,2,\ldots,n}\{\frac{\alpha_k}{\beta_k}\}(\sum_{i=1}^{m}\beta_i x_i - \prod_{i=1}^{m} x_i^{\beta_i}) \leq \sum_{i=1}^{m}\alpha_i x_i - \prod_{i=1}^{m} x_i^{\alpha_i} \leq \max_{k=1,2,\ldots,n}\{\frac{\alpha_k}{\beta_k}\}(\sum_{i=1}^{m}\beta_i x_i - \prod_{i=1}^{m} x_i^{\beta_i}). \quad (7)$$

Equality holds in either of the inequalities if and only if either $x_1 = \cdots = x_n$ or $\alpha_{max} = \beta_{min}$ (or equivalently, $\alpha_{min} = \beta_{max}$).

Theorem 2.4. *Let G be a graph with n vertices, m edges and z_i for $i = 1, 2, \ldots, m$ be the measures of its d-points w_i. Then*

$$\frac{1}{\beta_{max}}(\sum_{i=1}^{m}\beta_i z_i - \prod_{i=1}^{m} z_i^{\beta_i}) + mR_g \leq SO(G) \leq \frac{1}{\beta_{min}}(\sum_{i=1}^{m}\beta_i z_i - \prod_{i=1}^{m} z_i^{\beta_i}) + mR_g \quad (8)$$

such that $\beta = (\beta_1, \beta_2, \ldots, \beta_m)$, $\beta_i > 0$ and $\sum_{i=1}^{m} \beta_i = 1$. Equality holds in each of the inequalities if and only if $z_1 = z_2 = \ldots = z_m$ or $\beta_{max} = \frac{1}{m}$ (or $\beta_{min} = \frac{1}{m}$).

Proof. In Inequation (7), by setting $\alpha = (\alpha_1, \ldots, \alpha_m) = (\frac{1}{m}, \frac{1}{m}, \ldots, \frac{1}{m})$, it follows that

$$\frac{1}{m\beta_{max}}(\sum_{i=1}^{m}\beta_i z_i - \prod_{i=1}^{m} z_i^{\beta_i}) \leq \sum_{i=1}^{m}\frac{1}{m}z_i - \prod_{i=1}^{m} z_i^{\frac{1}{m}} \leq \frac{1}{m\beta_{min}}(\sum_{i=1}^{m}\beta_i z_i - \prod_{i=1}^{m} z_i^{\beta_i}),$$

thus

$$\frac{1}{\beta_{max}}(\sum_{i=1}^{m}\beta_i z_i - \prod_{i=1}^{m} z_i^{\beta_i}) \leq SO(G) - mR_g \leq \frac{1}{\beta_{min}}(\sum_{i=1}^{m}\beta_i z_i - \prod_{i=1}^{m} z_i^{\beta_i}),$$

and in result

$$\frac{1}{\beta_{max}}(\sum_{i=1}^{m}\beta_i z_i - \prod_{i=1}^{m} z_i^{\beta_i}) + mR_g \leq SO(G) \leq \frac{1}{\beta_{min}}(\sum_{i=1}^{m}\beta_i z_i - \prod_{i=1}^{m} z_i^{\beta_i}) + mR_g.$$

□

Definition 2.5. *[2] The variance of a vector of the real numbers $\mathbf{X}^{\frac{1}{2}} = (x_1^{\frac{1}{2}}, x_2^{\frac{1}{2}}, \ldots, x_m^{\frac{1}{2}})$ is defined as $\sigma^2(\mathbf{X}^{\frac{1}{2}}) = \frac{1}{m}\sum_{i=1}^{m}(x_i^{\frac{1}{2}} - \sum_{k=1}^{m}\frac{1}{m}x_k^{\frac{1}{2}})^2$ with respect to the discrete probability $\sum_{i=1}^{n}\alpha_i\delta_{x_i}$.*

Definition 2.6. *[24] For the nonnegative real numbers $X = \{x_1, x_2, \cdots, x_m\}$ the standard deviation is defined as $\sigma(X) = \sqrt{\sigma^2(X)}$.*

The standard deviation measures the amount of variation or dispersion in a set of values. In a graph, it shows how much the degrees of the vertices in a graph deviate from the average (mean) degree.

Definition 2.7. *Suppose $W = \{w_1, w_2, \ldots, w_m\}$ be the degree points related the edges of the graph G, then for the nonnegative numbers $Z = \{z_1, z_2, \ldots, z_m\}$ the arithmetic mean μ and variance σ^2 are denoted as:*

$$\mu(Z) = \frac{1}{m}\sum_{i=1}^{n} z_i = \frac{SO(G)}{m}, \quad \sigma^2(Z) = \frac{1}{m}\sum_{i=1}^{m}(z_i - \mu)^2 = \frac{1}{m}\sum_{i=1}^{m}(z_i - \frac{SO(G)}{m})^2. \tag{9}$$

Theorem 2.8. *[3, Th, 1] For $i = 1, 2, \ldots, m$, let $x_i \geq 0$, and let $\alpha_i > 0$ satisfy $\sum_{i=1}^{m} \alpha_i = 1$. Then*

$$\prod_{i=1}^{m} x_i^{\alpha_i} \leq \sum_{i=1}^{m} \alpha_i x_i - \sum_{i=1}^{m} \alpha_i (x_i^{\frac{1}{2}} - \sum_{k=1}^{m} \alpha_k . x_k^{\frac{1}{2}})^2. \tag{10}$$

Note that the right most term of Inequality (10) is the variance $var(\mathbf{x}^{\frac{1}{2}})$ of the vector

$$\mathbf{X}^{\frac{1}{2}} = (x_1^{\frac{1}{2}}, x_2^{\frac{1}{2}}, \ldots, x_m^{\frac{1}{2}})$$

with respect to the probability $\sum_{i=1}^{n} \alpha_i \delta_{x_i}$. So a large variance (of $\mathbf{x}^{\frac{1}{2}}$) pushes the arithmetic and geometric means apart.

Theorem 2.9. *Let G be a graph with n vertices and m edges such that for $i = 1, 2, \ldots, m$, z_i be the meaures of the degree-points w_i of G. Let $\alpha_i > 0$ satisfy $\sum_{i=1}^{m} \alpha_i = 1$. Then*

$$m(R_g + \sigma^2(\mathbf{Z}^{\frac{1}{2}})) \leq SO(G), \tag{11}$$

in which $\mathbf{Z}^{\frac{1}{2}} = (z_1^{\frac{1}{2}}, z_2^{\frac{1}{2}}, \ldots, z_m^{\frac{1}{2}})$.

Proof. It is clear that the right-hand of Inequality (10) is the variance of the set $\mathbf{X}^{\frac{1}{2}}$. Now consider the graph G with d-points w_i for $i = 1, 2, \ldots, m$, with $|w_i| = z_i$, and for $\alpha_i = \frac{1}{m}$, then we obtain

$$\prod_{i=1}^{m} z_i^{\frac{1}{m}} \leq \sum_{i=1}^{m} \frac{1}{m} z_i - \sum_{i=1}^{m} \frac{1}{m}(z_i^{\frac{1}{2}} - \sum_{k=1}^{m} \frac{1}{m} z_k^{\frac{1}{2}})^2.$$

Hence

$$m\prod_{i=1}^{m} z_i^{\frac{1}{m}} \leq \sum_{i=1}^{m} z_i - \frac{m}{m}\sum_{i=1}^{m}(z_i^{\frac{1}{2}} - \sum_{k=1}^{m} \frac{1}{m} z_k^{\frac{1}{2}})^2.$$

This implies that

$$mRg \leq SO(G) - m\sigma^2(\mathbf{Z}^{\frac{1}{2}}) \Rightarrow m(R_g + \sigma^2(\mathbf{Z}^{\frac{1}{2}})) \leq SO(G).$$

□

Remark 2.10. *[3] For $i = 1, 2, \ldots, m$, let $x_i \geq 0$, and let $\alpha_i > 0$ satisfy $\sum_{i=1}^{m} \alpha_i = 1$. Let $0 < M_1 = min\{x_1, x_2, \ldots, x_m\}$ and $M_2 = max\{x_1, x_2, \ldots, x_m\}$. Then*

$$\frac{1}{2M_2}\sum_{i=1}^{m} \alpha_i(x_i - \sum_{k=1}^{m} \alpha_k x_k)^2 \leq \sum_{i=1}^{m}\alpha_i x_i - \prod_{i=1}^{m} x_i\alpha_i \leq \frac{1}{2M_1}\sum_{i=1}^{m} \alpha_i(x_i - \sum_{k=1}^{m} \alpha_k x_k)^2.$$

Theorem 2.11. *Let G be a graph with n vertices, m edges. Consider $Z = \{z_1, z_2, \ldots, z_m\}$, $M_1 = min\{z_1, z_2, \ldots, z_m\}$ and $M_2 = max\{z_1, z_2, \ldots, z_m\}$. Then*

$$m(R_g + \frac{\sigma^2(Z)}{2M_2}) \leq SO(G) \leq m(R_g + \frac{\sigma^2(Z)}{2M_1}). \tag{12}$$

Proof. With attention to the Remark (2.10), considering the graph G with d-points w_i for $i = 1, 2, \ldots, m$. and for $z_i = |w_i|$ and $\alpha = (\alpha_1, \alpha_2, \ldots, \alpha_m) = (\frac{1}{m}, \frac{1}{m}, \ldots, \frac{1}{m})$, where $\sum_{i=1}^{m} \alpha_i = 1$, we have

$$\frac{1}{2M_2}\sum_{i=1}^{m} \frac{1}{m}(z_i - \sum_{k=1}^{m} \frac{1}{m}z_k)^2 \leq \sum_{i=1}^{m} \frac{1}{m}z_i - \prod_{i=1}^{m} z_i^{\frac{1}{m}} \leq \frac{1}{2M_1}\sum_{i=1}^{m} \frac{1}{m}(z_i - \sum_{k=1}^{m} \frac{1}{m}z_i)^2.$$

Thus

$$\frac{m}{2M_2 m}\sum_{i=1}^{m} (z_i - \sum_{k=1}^{m} \frac{1}{m}z_k)^2 \leq \sum_{i=1}^{m} z_i - m\prod_{i=1}^{m} z_i^{\frac{1}{m}} \leq \frac{m}{2M_1 m}\sum_{i=1}^{m} (z_i - \sum_{k=1}^{m} \frac{1}{m}z_i)^2$$

and so

$$\frac{m}{2M_2}\sigma^2(Z) \leq SO(G) - mR_g \leq \frac{m}{2M_1}\sigma^2(Z).$$

Consequently

$$m(R_g + \frac{\sigma^2(Z)}{2M_2}) \leq SO(G) \leq m(R_g + \frac{\sigma^2(Z)}{2M_1}).$$

□

Incorporating standard deviation into the Sombor index allows for the quantification of the degree-radius distribution's variability, providing a clearer understanding of how the degree-radii vary across the graph and its impact on topological properties.

Lemma 2.12. *[23] Let $m \geq 2$ and $x_1, x_2, \ldots, x_m$ be a sequance of $n \geq 2$ real numbers with mean $\mu > 0$ and variance σ^2.*

(a) If $0 \leq \frac{\sigma}{\mu} < \frac{1}{\sqrt{n-1}}$, then each x_i is positive.

(b) If every term of the sequence $x_1, x_2, \ldots, x_m$ is positive, then $0 \leq \frac{\sigma}{\mu} < \sqrt{m-1}$.

Corollary 2.13. *[23] Fix $m \geq 2$. If $x_1, x_2, \ldots, x_m$ is a positive sequence with mean μ and variance σ^2, then*

$$\mu - \sqrt[m]{x_1 \cdot x_2 \cdot \ldots \cdot x_m} \leq \sqrt{m-1}\,\sigma$$

Theorem 2.14. *Let $z_1, z_2, \ldots, z_m$ be a sequance of measures of degree-points $w_1, w_2, \ldots, w_m$ pertained edges of the graph G for $m \geq 2$. Then for the sequence $z_1, z_2, \ldots, z_m$ with $SO(G) > 0$ and variance σ^2, we obtain*

$$\frac{m}{\sqrt{m-1}}\sigma < SO(G) \leq m(R_g + \sqrt{m-1}\,\sigma). \tag{13}$$

Proof. By [23, Lemma, 2.10], whereas all of the terms of the sequence $z_1, z_2, \ldots, z_m$ are positive. So

$$\frac{\sigma}{\mu} < \sqrt{m-1}.$$

But $\mu = \frac{1}{m}\sum_{i=1}^{n} z_i = \frac{SO(G)}{m}$ and thus, after replacing the above inequation, the left inequation (13) is obtained. On the right hand, we can apply the Corollary (2.13) in reference [23], whereas all of the terms of the sequence $z_1, z_2, \ldots, z_m$ are positive, which yields that

$$\mu - \sqrt[m]{z_1 \cdot z_2 \cdot \ldots \cdot z_m} \leq \sqrt{m-1}\,\sigma.$$

Again $\mu = \frac{1}{m}\sum_{i=1}^{n} z_i = \frac{SO(G)}{m}$ and replacing in the above inequation, the right inequation is obtained. □

Definition 2.15. *The arithmetic-harmonic mean inequality for nonnegative real numbers $x_1, x_2, x_3, \ldots, x_m$ is as follow*

$$R_h = \frac{m}{\sum_{i=1}^{m} \frac{1}{x_i}} \leq \frac{1}{m}\sum_{i=1}^{m} x_i = R_a.$$

Using this inequality, we get the following theorem.

Theorem 2.16. *Let G be a graph with n vertices and m edges such that w_i for $i = 1, 2, \ldots, m$ be degree-points pertained edges. Then for the nonnegative numbers $z_1, z_2, \ldots, z_m$,*

$$mR_h \leq SO(G),$$

and the equality holds whenever $z_1 = z_2 = \ldots = z_m$.

In Theorem 2.28, $\lim_{m\to\infty} \frac{mR_g}{SO(G)}$ is calculated in random graphs.

In Example 3.1, the upper and lower bounds, expressed in terms of β_i, are adjusted by varying the β vector, and the conditions relative to the Sombor index are evaluated.

In [7], the well-known bounds for the Sombor index based on the minimum (δ) and the maximum (Δ) degree introduce as $\frac{\sqrt{2}n\delta^2}{2} \leq SO(G) \leq \frac{\sqrt{2}n\Delta^2}{2}$. This algebraic approach gives a general estimate of the Sombor index, but it does not give the finer structural details of the graph or does not reflect the degree distribution throughout the graph. Therefore, while it is useful as a big approximation, it may overestimate the Sombor index, especially in graphs where the degrees vary significantly across vertices.

The *triangle inequality* and *Cauchy-Schwarz inequality* are two key tools in deriving upper and lower bounds for the Sombor index of a graph. They provide a geometric perspective on degree of vertices, particularly through the Euclidean distance between degree-points of edges in a graph.

As one can see the distance between two d-points $w_1 = (d(u_1), d(v_1))$ and $w_2 = (d(u_2), d(v_2))$ is

$$|w_1 - w_2| = \sqrt{(d(u_1) - d(u_2))^2 + (d(v_1) - d(v_2))^2}$$

and it gives us a lower bound for the sum of absolute values of degree-points and states that for any two points in the degree-coordinate, the distance between them is less than or equal to the sum of the distances from each point to a third point. In mathematical terms, the *triangle inequality* is expressed as, $|w_1 + w_2| \leq |w_1| + |w_2|$. It can be generalized to more than two points, $w_1, w_2, \ldots, w_m$ as $|w_1 + w_2 + \ldots + w_m| \leq |w_1| + |w_2| + \ldots + |w_m|$ for $m = 2, 3, \cdots$.

The basis for obtaining many upper bounds in various areas of mathematics is the Cauchy-Schwarz inequality. We find an upper bound by it for the Sombor index of the graph G.

The Cauchy-Schwarz inequality for real numbers x_i and y_i $(i = 1, 2, \ldots, n)$ is stated as

$$(\sum_{i=1}^{m} x_i y_i)^2 \leq (\sum_{i=1}^{m} x_i^2).(\sum_{i=1}^{m} y_i^2) \tag{14}$$

and for two increasing sequences $\{x_i\}_{i=1}^{n}$ and $\{y_i\}_{i=1}^{n}$ is stated as

$$(\sum_{i=1}^{m} x_i)(\sum_{i=1}^{m} y_i) \leq m \sum_{i=1}^{m} x_i y_i. \tag{15}$$

Theorem 2.17. *Let G be a connected graph with n vertices and m edges. Then*

$$|w_1 + w_2 + \ldots + w_m| \leq SO(G) \leq \sum_{i=1}^{m} \sqrt{2(z_i^2 - d(u_i)d(v_i))},$$

where $w_1, w_2, \ldots, w_m$ are the degree-points for all edges in the graph.

Proof. Based on the triangle inequality and its generalization

$$\begin{aligned} SO(G) &= \sum_{uv \in E(G)} \sqrt{d^2(u) + d^2(v)} = z_1 + z_2 + \ldots + z_m \\ &= |w_1| + |w_2| + \ldots + |w_m| \geq |w_1 + w_2 + \ldots + w_m|. \end{aligned}$$

For the right inequality, using (2), $(d(u) + d(v))^2 \leq (\sqrt{2}|w|)^2 = (\sqrt{2}z)^2$ and hence

$$d^2(u) + d^2(v) \leq 2z^2 - 2d(u)d(v),$$

which implies $SO(G) \leq \sum_{i=1}^{m} \sqrt{2(z_i^2 - d(u_i)d(v_i))}$.

□

Theorem 2.18. *Let $w_1, w_2, \ldots, w_m$ be d-points of graph G_1 with Euclidean distances $z_1 > z_2 > \ldots > z_m$ and $s_1, s_2, \ldots, s_m$ be d-points of graph G_2 with Euclidean distances $z'_1 > z'_2 > \ldots > z'_m$. Then*

$$\sum_{i=1}^{m} z_i.\, z'_i \leq SO(G_1).SO(G_2) \leq m \sum_{i=1}^{m} z_i.\, z'_i.$$

Proof. For the left-hand inequality, consider $a_i = \sqrt[4]{d^2(u) + d^2(v)}$ in G_1. Then $z_i = a_i^2 = (\sqrt[4]{d^2(u) + d^2(v)})^2 = \sqrt{d^2(u) + d^2(v)}$ and in result $\sum_{i=1}^{m} z_i = \sum_{i=1}^{m} a_i^2 = SO(G_1)$ and in G_2 consider $b_i = \sqrt[4]{d^2(\overline{u}) + d^2(\overline{v})}$, then $z'_i = b_i^2 = (\sqrt[4]{d^2(\overline{u}) + d^2(\overline{v})})^2 = \sqrt{d^2(u) + d^2(v)}$ and in result $\sum_{i=1}^{m} z'_i = \sum_{i=1}^{m} b_i^2 = SO(G_2)$. Based on the above relations and Inequality (14), we have

$$\begin{aligned}\sum_{i=1}^{m} z_i.z'_i &\leq (\sum_{i=1}^{m} (z_i.{z'}_i)^{\frac{1}{2}})^2 = (\sum_{i=1}^{m} z_i^{\frac{1}{2}}.{z'}_i^{\frac{1}{2}})^2 = (\sum_{i=1}^{m} a_i b_i)^2 \leq (\sum_{i=1}^{m} a_i^2)(\sum_{i=1}^{m} b_i^2)\\ &= (\sum_{i=1}^{m} \sqrt{d^2(u) + d^2(v)})(\sum_{i=1}^{m} \sqrt{d^2(u) + d^2(v)})\\ &= SO(G_1).SO(G_2).\end{aligned}$$

For the right-hand inequality, by inequality (15), it is concluded that for the nonnegative numbers z_i and z'_i $(i = 1, 2, \ldots, m)$ if $z_1 > z_2 > \ldots > z_m$ and $z'_1 > z'_2 > \ldots > z'_m$, then

$$(\sum_{i=1}^{m} z_i)(\sum_{i=1}^{m} z'_i) \leq m \sum_{i=1}^{m} z_i.\, z'_i \Rightarrow SO(G_1).SO(G_2) \leq m \sum_{i=1}^{m} z_i.\, z'_i.$$

Therefore

$$\sum_{i=1}^{m} z_i.\, z'_i \leq SO(G_1).SO(G_2) \leq m \sum_{i=1}^{m} z_i.\, z'_i.$$

□

Definition 2.19. *[5] If $f : \mathbb{R}^n \to \mathbb{R}$ is a norm, and $0 \leq \theta \leq 1$, then*

$$f(\theta x + (1-\theta)y) \leq f(\theta x) + f((1-\theta)y) = \theta f(x) + (1-\theta) f(y),$$

is named Jensen's inequality and it follows from the triangle inequality, and the equality follows from the homogeneity of a norm.
The inequality extends to infinite sums, integrals, and expected values.

Definition 2.20. *[5] Assume that f is twice differentiable, that is, second derivative $\nabla^2 f$ exists at each point in **dom** f, which is open, then*

*1. f is convex if and only if its **dom** is convex and second derivative $\nabla^2 f(x) \geq 0$ (positive semidefinite) for all $x \in$ **dom**f. For functions on R, this reduces to $f''(x) \geq 0$, implying the derivative is nondecreasing.*

*2. Similarly, f is concave if $\nabla f(x) \leq 0$ for all $x \in$ **dom**f. Strict convexity can be partially characterized by the condition $\nabla^2 f(x) > 0$, although the converse is not always true.*

Theorem 2.21. *Let G be a graph with the $Z = \{z_1, z_2, \ldots, z_m\}$ and the Sombor index $SO(G)$. Then*

$$SO(G) = \sum_{i=1}^{m} z_i \leq m \cdot \left(\frac{1}{m} \sum_{i=1}^{m} z_i^r \right)^{1/r}, \tag{16}$$

in which $\left(\frac{1}{m} \sum_{i=1}^{m} z_i^r \right)^{1/r}$ is named generalized mean or power mean and displayed by $M_r(z_1, z_2, \ldots, z_m)$.

Proof. Given G be a graph with the degree points $W = \{w_1, w_2, \cdots, w_m\}$ and Euclidean distances $Z = \{z_1, z_2, \ldots, z_m\}$, formed by $z_i = |w_i| = \sqrt{d(u)^2 + d(v)^2}$ then it is aimed to bound $SO(G)$ using Jensen's inequality. For this means, it is proved that the function $f(w_i) = |w_i|^r = z_i^r$ is convex, where $z_i = |w_i| = \sqrt{d(u_i)^2 + d(v_i)^2}$ is the Euclidean norm for $r \geq 2$. Therefore, it is proved that $f''(w_i)$ is nonnegative. For simplicity, the function is rewriting as $f(w_i) = \left(d(u_i)^2 + d(v_i)^2\right)^{r/2}$. This can be treated as the function $f(x) = x^{r/2}$, where $x = d(u_i)^2 + d(v_i)^2$. Thus, the convexity of $f(x) = x^{r/2}$ is equivalent to proving the convexity of $f(w_i) = |w_i|^r = z_i^r$. The convexity condition is given by using second derivative $f(x) = x^{r/2}$. So, $f'(x) = \frac{r}{2} x^{(r/2)-1}$, then $f''(x) = \frac{r}{2} \cdot \left(\frac{r}{2} - 1\right) x^{(r/2)-2}$ (the function $f(x) = x^{r/2}$ is convex if $f''(x) \geq 0$ for all $x \geq 0$). For $r \geq 2$, we have $\frac{r}{2} - 1 \geq 0$, which means the second derivative is nonnegative for all $x \geq 0$. Thus, $f''(x) = \frac{r}{2} \cdot \left(\frac{r}{2} - 1\right) x^{(r/2)-2} \geq 0$. So, the function $f(w_i) = |w_i|^r = z_i^r$, where $z_i = |w_i| = \sqrt{d(u_i)^2 + d(v_i)^2}$, is convex.

Now, Jensen's inequality states that for a convex function $f(x)$, the function evaluated at the mean is less than or equal to the mean of the function, in other words, $f(\frac{1}{m} \sum_{i=1}^{m} x_i) \leq \frac{1}{m} \sum_{i=1}^{m} f(x_i)$. Applying Jensen's inequality to the convex function $f(w_i) = |w_i|^r = z_i^r$, and for $r \geq 2$ we have:

$$\left(\frac{1}{m} \sum_{i=1}^{m} z_i \right)^r \leq \frac{1}{m} \sum_{i=1}^{m} z_i^r.$$

Now taking the r-th root on both sides, we obtain

$$\frac{1}{m} \sum_{i=1}^{m} z_i \leq \left(\frac{1}{m} \sum_{i=1}^{m} z_i^r \right)^{1/r}$$

and thus

$$\sum_{i=1}^{m} z_i \leq m. \left(\frac{1}{m} \sum_{i=1}^{m} z_i^r \right)^{1/r}.$$

Finally, we have

$$SO(G) \leq m \cdot M_r(z_1, z_2, \ldots, z_m). \tag{17}$$

□

Note that in the inequality 16, if $r = 2$, it takes the form $SO(G) \leq \sqrt{mF(G)}$, which is satated in the inequality 6.

Now we are going to present some concepts related to random variables. A *random variable*, see [28], is a real-valued function defined over a sample space. A random variable Z is said to be *discrete* if it can assume only a finite or countably infinite number of distinct values. A random variable Z that can take on any value in an interval is called a *continuous* random variable.

Definition 2.22 (Expected value). *[16] If Z is a discrete random variable and $f(z)$ is the value of its probability distribution at z, the expected value of Z is $E[Z] = \sum_z z \cdot f(z)$. Correspondingly, if Z is a continuous random variable and $f(z)$ is the value of its probability density at z, the expected value of Z is $E[Z] = \int_{-\infty}^{\infty} z \cdot f(z)$.*

Definition 2.23 (Standard distribution). *[16] If the random variable Z has the mean μ and the standard deviation σ, then the random variable X whose values are related to those of Z by means of the equation $x = \frac{z-\mu}{\sigma}$ has $E(X) = 0$ and $var(X) = 1$. A distribution that has the mean 0 and the variance 1 is said to be in standard form, and when we perform the above change of variable, we are said to be standardizing the distribution of Z.*

Theorem 2.24 (Standardized Sombor index). *Let G be a graph with m edges, and $Z(w_i) := \sqrt{d(u_i)^2 + d(v_i)^2}$ be the random variable related to the graph as degree-points $w_i = (d(u_i), d(v_i))$. Define the standardized values of z_i as $x_i = \frac{z_i-\mu}{\sigma}$. Then the standardized Sombor index $SO_{st}(G) = \sum_{i=1}^{m} x_i$ satisfies the following inequality*

$$SO_{st}(G) = \sum_{i=1}^{m} x_i \leq m. \left(\frac{1}{m} \sum_{i=1}^{m} x_i^r \right)^{1/r} = m \cdot M_r(x_1, x_2, \ldots, x_m).$$

Proof. By substituting x_i in inequality (16), the proof is clear. □

Theorem 2.25 (Mean Sombor index). *Let G be a graph with m edges, Z be the random variable related to the graph and μ be mean of z_i's. Define the standardized values of z_i as $x_i = \frac{z_i-\mu}{\sigma}$, where μ is the mean of the z_i's and σ is their standard deviation. Then the mean Sombor index $SO_\mu(G) := \sum_{i=1}^{m} |z_i - \mu|$ satisfies the following inequality:*

$$SO_\mu(G) = \sum_{i=1}^{m} |z_i - \mu| \leq m \cdot \left(\frac{1}{m} \sum_{i=1}^{m} |z_i - \mu|^r \right)^{1/r} = m \cdot M_r(z_1 - \mu, z_2 - \mu, \ldots, z_m - \mu)$$

Proof. Starting from the generalized mean inequality for the standardized variables and by Jensen's inequality:

$$\left(\frac{1}{m} \sum_{i=1}^{m} x_i \right)^r \leq \frac{1}{m} \sum_{i=1}^{m} x_i^r.$$

Substituting $x_i = \frac{z_i-\mu}{\sigma}$, we obtain

$$\left(\frac{1}{m}\sum_{i=1}^{m}|\frac{z_i-\mu}{\sigma}|\right)^r \leq \frac{1}{m}\sum_{i=1}^{m}|\frac{z_i-\mu}{\sigma}|^r.$$

Now, simplifying both sides:

- The left-hand side becomes:

$$\left(\frac{1}{m}\sum_{i=1}^{m}\frac{|z_i-\mu|}{\sigma}\right)^r = \frac{1}{\sigma^r}\left(\frac{1}{m}\sum_{i=1}^{m}|z_i-\mu|\right)^r.$$

-The right-hand side becomes:

$$\frac{1}{m}\sum_{i=1}^{m}\left(\frac{|z_i-\mu|}{\sigma}\right)^r = \frac{1}{\sigma^r}\cdot\frac{1}{m}\sum_{i=1}^{m}|z_i-\mu|^r.$$

Now substituting back,

$$\frac{1}{\sigma^r}\left(\frac{1}{m}\sum_{i=1}^{m}|z_i-\mu|\right)^r \leq \frac{1}{\sigma^r}\cdot\frac{1}{m}\sum_{i=1}^{m}|z_i-\mu|^r$$

Multipling both sides by σ^r (assuming $\sigma \neq 0$):

$$\left(\frac{1}{m}\sum_{i=1}^{m}|z_i-\mu|\right)^r \leq \frac{1}{m}\sum_{i=1}^{m}|z_i-\mu|^r.$$

Finally, taking the $r-$th root of both sides results in

$$\frac{1}{m}\sum_{i=1}^{m}|z_i-\mu| \leq \left(\frac{1}{m}\sum_{i=1}^{m}|z_i-\mu|^r\right)^{\frac{1}{r}}$$

and in result,

$$SO_\mu(G) \leq m\cdot\left(\frac{1}{m}\sum_{i=1}^{m}|z_i-\mu|^r\right)^{\frac{1}{r}}.$$

Therefore, the mean Sombor index, $SO_\mu(G)$, is less than or equal to the $r-$th root of the mean of the $r-$th powers of the absolute deviations, $|z_i-\mu|$, scaled by the coefficient m for all i from 1 to m. □

A powerful tool for solving many problems in discrete mathematics is the probabilistic method. In this method, it tried to prove certain desired properties for a structure hold by defining an appropriate probability with positive probability. An active area of research that combines probability theory and graph theory is the area of *random graphs*.

Based on the [15], a random graph is generated by a random procedure formalized through a probability space (Ω, F, P), and its distribution refers to the induced probability distribution on the family of graphs. Graphs with the same distribution are usually considered equivalent. For the study of random graphs, two basic models have introduced: the binomial model and the uniform model, both rooted in the simple model was introduced by Erdös (1947).

The *binomial random graph* $G(n,p)$ is defined on n vertices where each possible edge between vertex pairs happens independently with probability p and the probability of observing a particular graph G with m edges is $P(G) = p^m(1-p)^{\binom{n}{2}-m}$. It is often interpreted as the result of an independent coin flips for each vertex pair of edge inclusion. The number of edges is based on a binomial distribution with expected value $\binom{n}{2}p$. In this model of graphs, the number of edges is not fixed and independence edges is the main advantage of the binomial model $G(n,p)$.

In the *uniform random graph* model $G(n,M)$, where a graph is chosen uniformly at random from the set of all graphs with n vertices and exactly M edges. The probability of selecting any specific graph G with M edges from this space is $\binom{\binom{n}{2}}{M}^{-1}$. The number of edges in this model directly fixed at M.

There are other models for the random graphs which aren't in these models (binomial or uniform). A stochastic process where a graph evolves over time by adding edges is named a *random graph process*, either in discrete or continuous time, without removing any. The graph starts with no edges and grows according to predefined rules on a fixed vertex set.

A well-known *random graph process* introduced by Erdös-Rényi (1959). It starts with no edges and adds new edges uniformly at random, one at a time. This process is a *Markov process* where the $M-$th stage corresponds to the uniform random graph $G(n,M)$, with M edges.

The *Continuous time random graph process* assigns a random variable T_e to each edge e of the complete graph K_n, where the $\binom{n}{2}$ variables T_e are independent and follow a *common continuous distribution* and then define the adge set $\{G(t)\}_t$ containing of all e with $T_e \leq t$. The resulting random graph $\{G(t)\}_{t_0}$ in a fix point t_0 is identified with the binomial random graph $G(n,p)$ with $p = P(T_e \leq t)$.

Also, no two values of the random variables T_e as almost surly coincide, we may define $T_{(i)}$ as the random time at which the $i-$th edge is added. Then, by symmetry, $G(T_i)$ is the uniform random graph $G(n,i)$, and the sequence $G(T_i)$ for $i = 1,\cdots,\binom{n}{2}$, equals the ordinary random graph process $G(n,M)_M$ defined above. Hence, this continuous time random graph process is a joint generalization of the binomial random graph, the uniform random graph and the standard discrete-time random graph process. Clearly, different choices of the distribution of T_e affect the model only trivially, by a change in the time variable. The continuous time evolving model was introduced by Stepanov (1970) with T_e exponentially distributed; we prefer the uniform distribution over the interval $[0,1]$, in which case $p = P(T_e \leq t) = t, 0 \leq t \leq 1$. Thus, we may unambiguously use the notation $G(n,t)_t$.

Now, we state Theorem (2.28) about the Sombor index of random graphs with continuous time random graph process, but previous of it we state some nesseserlies:

Lemma 2.26 (The weak law of large numbers (LLN)). *[24] Let Z_1, Z_2, $\cdots$, Z_m be a sequence of independent and identically distributed (i.i.d) random variables, each having finite mean $E(Z_i) = \mu$.*

Then, for any $\epsilon > 0$, $\lim_{m\to\infty} P(\frac{Z_1+Z_2+...+Z_m}{m} - \mu \geq \epsilon) = 0$.

Definition 2.27 (Euler's constant). *[19] Constant* γ *discoverd by Euler, defined by* $\gamma := \lim_{n\to\infty}(\sum_{j=1}^{n}\frac{1}{j} - \log n)$ *and called Euler's constant. It is to* 50 *decimal places as*

$$\gamma = 0.57721566490153286060651209008240243104215933593992\cdots$$

and as well $e^{-\gamma} = 0.561459\cdots$.

Theorem 2.28. *Let* $G(n,p)$ *be a random Erdös-Rényi graph with n vertices and m edges, where each edge exists independently with probability p. The waiting time for the creation of each edge follows countinuous time random graph process. Then, as* $m \to \infty$*, we have the following convergence result*

$$\lim_{m\to\infty} r_m(Z) = e^{-\gamma},$$

where $r_m(Z) = \frac{mR_g}{SO(G)}$, R_g *is the geometric mean of* z_i*'s and* γ *is the Euler's constant.*

Proof. Since the waiting time for the creation of each edge follows a continuous time random graph process, so we could use the exponential distribution with rate parameter λ, the probability density function of Z with $f_\lambda(z) = \lambda e^{-\lambda z}, z > 0$ and the expected value of Z, $E[Z] = \frac{1}{\lambda}$.

At first, compute the expected value of the logarithm of Z, i.e., $E[lnZ]$. This is calculated as:

$$E[lnZ] = \int_0^\infty ln(z) f_Z(z) dz = \int_0^\infty ln(z)\lambda e^{-\lambda z} dz = \lambda \int_0^\infty ln(z) e^{-\lambda z} dz.$$

With considering a change of variable as $u = \lambda z$, $du = \lambda dz$, and thus $dz = \frac{du}{\lambda}$ the integral becomes:

$$\begin{aligned} E[lnZ] &= \lambda \int_0^\infty ln(\frac{u}{\lambda}) e^{-u} \frac{du}{\lambda} = \int_0^\infty (ln(u) - ln(\lambda)) e^{-u} du \\ &= \int_0^\infty (ln(u)) e^{-u} du - \int_0^\infty (ln(\lambda)) e^{-u} du \\ &= \int_0^\infty (ln(u)) e^{-u} du - ln(\lambda) = -\gamma - ln(\lambda). \end{aligned}$$

Hence

$$E[lnZ] = -\gamma - ln(\lambda),$$

where γ is Euler's constant (approximately 0.5772).

Now whereas $R_g = (\prod_{i=1}^{m} z_i)^{\frac{1}{m}} = exp(\frac{1}{m}\sum_{i=1}^{m} z_i)$, so $lnR_g = \frac{1}{m}\sum_{i=1}^{m} ln(z_i)$. By the law of large numbers, as $m \to \infty$, the average converges to the expected value:

$$\lim_{m\to\infty} P(|\frac{1}{m}\sum_{i=1}^{m} ln(z_i) - E[ln(Z)]| \geq \epsilon) = 0.$$

Thus

$$\lim_{m\to\infty} P(|\frac{1}{m}\sum_{i=1}^{m} ln(z_i) - E[ln(Z)]| < \epsilon) = 1$$

and so

$$\lim_{m\to\infty} P(|lnR_g - E[ln(Z)]| < \epsilon) = 1.$$

So, while $\epsilon > 0$ can be arbitrarily small, in the limit, the actual difference between the two is essentially zero with the probability 1. Therefore,

$$\begin{aligned}\lim_{m\to\infty} P(|lnR_g - E[ln(Z)]| < \epsilon) = 1 \text{ iff } \lim_{m\to\infty} P(|R_g - e^{E[ln(Z)]}| < \epsilon) = 1 \\ \text{iff } \lim_{m\to\infty} P(|R_g - e^{-\gamma - ln(\lambda)}| < \epsilon) = 1 \text{ iff } \lim_{m\to\infty} R_g = e^{-\gamma - ln(\lambda)} \\ \text{iff } \lim_{m\to\infty} R_g = \frac{e^{-\gamma}}{e^{ln(\lambda)}} \text{ iff } \lim_{m\to\infty} R_g = \frac{e^{-\gamma}}{\lambda}. \end{aligned} \tag{18}$$

Also by using again of the LLN

$$\begin{aligned}\lim_{m\to\infty} P(|\frac{1}{m}\sum_{i=1}^{m} z_i - E[Z]| \geq \epsilon) = 0 \text{ iff } \lim_{m\to\infty} P(|\frac{1}{m}\sum_{i=1}^{m} z_i - E[Z]| < \epsilon) = 1 \\ \text{iff } \lim_{m\to\infty} \frac{1}{m}\sum_{i=1}^{m} z_i = E[Z]. \end{aligned} \tag{19}$$

Now with attention to Equation (19), the $E[\sum_{i=1}^{m} z_i] = \sum_{i=1}^{m} E[z_i] = m.E[Z]$ and using LLN

$$\begin{aligned}\lim_{m\to\infty} P(|\sum_{i=1}^{m} z_i - mE[Z]| \geq \epsilon) = 0 \text{ iff } \lim_{m\to\infty} P(|SO(G) - mE[Z]| \geq \epsilon) = 0 \\ \text{iff } \lim_{m\to\infty} P(|SO(G) - mE[Z]| < \epsilon) = 1 \text{ iff } \lim_{m\to\infty} SO(G) = m.E[Z] \\ \text{iff } \lim_{m\to\infty} SO(G) = m\frac{1}{\lambda}. \end{aligned} \tag{20}$$

So by $r_m(z) = \frac{mR_g}{SO(G)}$, and Equations (18) and (20), it is resulted

$$\begin{aligned}\lim_{m\to\infty} P(|\frac{m.R_g}{SO(G)} - \frac{m.\frac{e^{-\gamma}}{\lambda}}{m.\frac{1}{\lambda}}| \geq \epsilon) = 0 \text{ iff } \lim_{m\to\infty} p\{|r_m(z) - e^{-\gamma}| \geq \epsilon\} = 0 \\ \text{iff } \lim_{m\to\infty} p(|r_m(z) - e^{-\gamma}| < \epsilon) = 1 \text{ iff } \lim_{m\to\infty} r_m(z) = e^{-\gamma}\end{aligned}$$

and hence,

$$\lim_{m\to\infty} r_m(z) = e^{-\gamma}.$$

□

As a final result at this part, we apply Markov's inequality to derive an inequality for the Sombor index:

Lemma 2.29 (Markov's inequality). *[16] If Z is a random variable with the mean μ for which $f(z) = 0$ (probability density function or probability distribution function of Z) for $z < 0$, then for any positive constant a,*

$$P(Z \geq a) \leq \frac{\mu}{a}.$$

Theorem 2.30. *Let G be a graph with the set of degree-radii $Z = \{z_1, z_2, \ldots, z_m\}$ as a random variable. Then for any positive constant a,*

$$P(Z \geq a) \leq \frac{SO(G)}{a.m}.$$

Proof. Whereas for the graph G with the random variable $Z = \{z_1, z_2, \cdots, z_m\}$, $f(z) = 0$ for $z < 0$, so it is enough to put $\mu = \frac{1}{m}\sum_{i=1}^{m} z_i = \frac{SO(G)}{m}$ in the Markov's inequality. □

Open Problem 2.31. *Consider a graph G with $m = 100$ edges, a known Sombor index $SO(G) = 300$ and the random variable $Z = \{z_1, z_2, \ldots, z_m\}$. Assume a positive constant $a = 5$. Determine the probability that Z is greater than or equal to a.*

Based on the theorem, we have:

$P(Z \geq a) \leq \frac{SO(G)}{a \cdot m} = \frac{300}{5 \cdot 100} = \frac{3}{5}$. *Thus, the probability that Z is greater than or equal to 5 is at most $\frac{3}{5}$.*

Now, we determine some bounds for the Sombor index by coefficients of the arithmetic-geometric and geometric-arithmetic indices applied in mathematical chemistry and you could see them in the articles [30], [8] and [6]. Also, in reference [29], the authors survey the correlation between the Sombor index and other degree-based topological indices.

Definition 2.32 (The arithmetic-geometric (AG) and geometric-arithmetic (GA) index). *Two important topological indices applied in the chemical graph theory and are stated in [6] and [26] are the AG index and GA index which are defined as follows,*

$$AG(G) = \sum_{uv \in E(G)} \frac{1}{2}\left(\sqrt{\frac{d(u)}{d(v)}} + \sqrt{\frac{d(v)}{d(u)}}\right) = \sum_{uv \in E(G)} \frac{1}{2}\left(\frac{d(u) + d(v)}{\sqrt{d(u)d(v)}}\right),$$

and

$$GA(G) = \sum_{uv \in E(G)} \left(\frac{2\sqrt{d(u)d(v)}}{d(u) + d(v)}\right).$$

Considering the reference [26], it is proved that

$$GA(G) \leq AG(G).$$

Also, note that

$$AG(G) \leq SO(G),$$

because for each edge $e = uv \in E(G)$,

$$\frac{d(u)+d(v)}{2\sqrt{d(u)d(v)}} \leq \frac{d(u)+d(v)}{2} \leq \frac{d(u)+d(v)}{\sqrt{2}} \leq \sqrt{d^2(u)+d^2(v)}.$$

So $\sum_{i=1}^{m} \frac{d(u)+d(v)}{2\sqrt{d(u)d(v)}} \leq \sum_{i=1}^{m} \sqrt{d^2(u)+d^2(v)}$ and hence $AG(G) \leq SO(G)$.

Now we are going to improve the above bound.

Theorem 2.33. *Let G be a graph with n vertices, m edges and with a maximum degree Δ and minimum degree δ, then*

$$\sqrt{2}\delta AG(G) \leq SO(G) \leq \sqrt{2}\Delta AG(G).$$

Proof. For obtaining the lower bound and upper bound, consider the following function

$$f(x,y) = \frac{\sqrt{x^2+y^2}}{\frac{x+y}{2\sqrt{xy}}} = \frac{2\sqrt{x^3y+y^3x}}{x+y}$$

where $1 \leq \delta \leq x,y \leq \Delta$. Therefore

$$\frac{\partial f}{\partial x} = \frac{(x^3y+y^3x)(3x^2y+y^3)(x+y) - 2\sqrt{x^3y+y^3x}}{(x+y)^2} \geq 0 \textit{ and also } \frac{\partial f}{\partial y} \geq 0.$$

It follows that $f(x,y)$ is an increasing function on the variables x and y. Thus, the function obtains its minimum at the point (δ,δ) and it's maximum at the point (Δ,Δ). It is concluded that

$$f(\delta,\delta) \leq f(x,y) \leq f(\Delta,\Delta) \Rightarrow \sqrt{2}\delta \leq f(x,y) \leq \sqrt{2}\Delta$$
$$\Rightarrow \sqrt{2}\delta\frac{x+y}{2\sqrt{xy}} \leq \sqrt{x^2+y^2} \leq \sqrt{2}\Delta\frac{x+y}{2\sqrt{xy}}$$

So for the set of edges $\{e_1 = u_1v_1, e_2 = u_2v_2, \cdots, u_mv_m\}$,

$$\sqrt{2}\delta\sum_{i=1}^{m}\frac{d_{u_i}+d_{v_i}}{2\sqrt{d_{u_i}d_{v_i}}} \leq \sum_{i=1}^{m}\sqrt{d_{u_i}^2+d_{v_i}^2} \leq \sqrt{2}\Delta\sum_{i=1}^{m}\frac{d_{u_i}+d_{v_i}}{2\sqrt{d_{u_i}d_{v_i}}}$$

and hence $\sqrt{2}\delta AG(G) \leq SO(G) \leq \sqrt{2}\Delta AG(G)$. □

Theorem 2.34. *Let G be a graph with n vertices and m edges, then*

$$GA(G) < SO(G).$$

Proof. Base on the Inequality (3) for each edge $e = uv \in E(G)$, $\sqrt{d(u).d(v)} \leq \frac{d(u)+d(v)}{2}$. So $\frac{2\sqrt{d(u).d(v)}}{d(u)+d(v)} \leq 1$, and since $\sqrt{d^2u+d^2v} > 1$,

$$\sum_{uv\in E(G)}\frac{2\sqrt{d(u).d(v)}}{d(u)+d(v)} < \sum_{uv\in E(G)}\sqrt{d^2(u)+d^2(v)} \Rightarrow GA(G) < SO(G).$$

□

Now we are going to improve this bound.

Theorem 2.35. *Let G be a graph with n vertices and m edges, then*

$$\sqrt{2}\delta GA(G) \leq SO(G) \leq \sqrt{2}(\Delta)GA(G)$$

Proof. Consider the following function

$$f(x,y) = \left(\frac{\sqrt{x^2+y^2}}{\frac{2\sqrt{xy}}{x+y}}\right)^2 = \frac{(x^2+y^2)(x+y)^2}{4xy},$$

where $2 \leq \delta \leq x \leq y \leq \Delta$. By using a proof similar to that of Theorem 2.33, the statement can be proven. □

Based on the reference [27], the symmetric division deg index (SDD(G)) is another index for predicting some physicochemical properties of substances, and the International Academy of Mathematical Chemistry carries out its test, so here we want to pay a little attention to it and compare it with Sombor index:

Definition 2.36 (The symmetric division deg index (SDD(G))). *For the graph G, the symmetric division deg index SDD(G) is defined as*

$$SDD(G) = \sum_{i=1}^{m}\left(\frac{d(u)}{d(v)} + \frac{d(v)}{d(u)}\right) = \sum_{i=1}^{m}\frac{d^2(u)+d^2(v)}{d(u)d(v)}.$$

Theorem 2.37. *Let G be a graph with n vertices and m edges, then*

$$\frac{\sqrt{2}}{2}\delta SDD(G) \leq SO(G) \leq \frac{\sqrt{2}}{2}\Delta SDD(G).$$

Proof. Consider the following function

$$f(x,y) = \frac{xy}{\sqrt{x^2+y^2}}$$

where $1 \leq \delta \leq x \leq y \leq \Delta$. Then $\frac{\partial f}{\partial x} \geq 0$ and $\frac{\partial f}{\partial x} \geq 0$. This means that $f(x,y)$ is an increasing function on x and y and gives its minimum at the point (δ,δ) and it's maximum at point (Δ,Δ). So $f(\delta,\delta) \leq f(x,y) \leq f(\Delta,\Delta)$ which deduces that

$$\frac{\sqrt{2}}{2}\delta\frac{x^2+y^2}{xy} \leq \sqrt{x^2+y^2} \leq \frac{\sqrt{2}}{2}(\Delta)\frac{x^2+y^2}{xy}$$
$$\Rightarrow \frac{\sqrt{2}}{2}\delta\sum_{i=1}^{m}\frac{x^2+y^2}{xy} \leq \sum_{i=1}^{m}\sqrt{x^2+y^2} \leq \frac{\sqrt{2}}{2}(\Delta)\sum_{i=1}^{m}\frac{x^2+y^2}{xy}.$$

Thus $\frac{\sqrt{2}}{2}\delta SDD(G) \leq SO(G) \leq \frac{\sqrt{2}}{2}\Delta SDD(G)$. □

3 Applications

Example 3.1. *Consider a simple graph G with 5 edges and 5 vertices as it is given in Figure (1). Assume that each edge is assigned a weight $\beta_i > 0$, such that $\sum_{i=1}^{m} \beta_i = 1$. Find the upper and lower bounds of $SO(G)$ in the following conditions:*

(i) *Using the inequalities derived from Theorem (2.4) and for*
$\beta = (0.2, 0.3, 0.2, 0.2, 0.1)$,
$\beta' = (0.1, 0.3, 0.2, 0.2, 0.2)$.

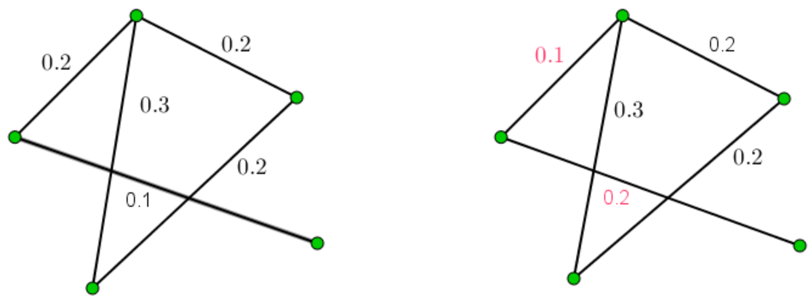

Figure 1. The weighted graph G with the edge weight vectors $\beta = (0.2, 0.3, 0.2, 0.2, 0.1)$ and $\beta' = (0.1, 0.3, 0.2, 0.2, 0.2)$.

For this means, first, we have

$$z_1 = z_2 = z_3 = \sqrt{13},\ z_4 = \sqrt{5},\ z_5 = \sqrt{8} \Rightarrow SO(G) = 3 \cdot \sqrt{13} + \sqrt{5} + \sqrt{8} = 15.88.$$

$$R_g = (\prod_{i=1}^{5} z_i)^{\frac{1}{5}} = (\sqrt{13} \cdot \sqrt{13} \cdot \sqrt{13} \cdot \sqrt{5} \cdot \sqrt{8})^{\frac{1}{5}} = 3.12, \Rightarrow 5 \cdot R_g = 15.61.$$

Now, for $\beta = (0.2, 0.3, 0.2, 0.2, 0.1)$:

$$\sum_{i=1}^{5} \beta_i z_i = 0.2 \cdot \sqrt{13} + 0.3 \cdot \sqrt{13} + 0.2 \cdot \sqrt{13} + 0.1 \cdot \sqrt{5} + 0.2 \cdot \sqrt{8} = 3.31,$$

$$\prod_{i=1}^{5} z_i^{\beta_i} = \sqrt{13}^{0.2} + \sqrt{13}^{0.3} + \sqrt{13}^{0.2} + \sqrt{5}^{0.1} + \sqrt{8}^{0.2} = 3.27,$$

so based on Theorem (2.4):

the lower bound is

$$\frac{1}{\beta_{max}}(\sum_{i=1}^{5} \beta_i z_i - \prod_{i=1}^{5} z_i^{\beta_i}) + 5 \cdot R_g = \frac{1}{0.3} \cdot (3.31 - 3.27) + 15.61 = 15.74, \tag{21}$$

and upper bound is

$$\frac{1}{\beta_{min}}(\sum_{i=1}^{5} \beta_i z_i - \prod_{i=1}^{5} z_i^{\beta_i}) + 5 \cdot R_g = \frac{1}{0.1} \cdot (3.31 - 3.27) + 15.61 = 16.01. \tag{22}$$

Now consider $\beta' = (0.1, 0.3, 0.2, 0.2, 0.2)$:

$$\sum_{i=1}^{5} \beta_i z_i = 0.1 \cdot \sqrt{13} + 0.3 \cdot \sqrt{13} + 0.2 \cdot \sqrt{13} + 0.2 \cdot \sqrt{5} + 0.2 \cdot \sqrt{8} = 3.18,$$

$$\prod_{i=1}^{5} z_i^{\beta_i} = \sqrt{13}^{0.1} + \sqrt{13}^{0.3} + \sqrt{13}^{0.2} + \sqrt{5}^{0.2} + \sqrt{8}^{0.2} = 3.12,$$

so based on Theorem (2.4), the lower bound is

$$\frac{1}{\beta_{max}}(\sum_{i=1}^{5} \beta_i z_i - \prod_{i=1}^{5} z_i^{\beta_i}) + 5 \cdot R_g = \frac{1}{0.3} \cdot (3.18 - 3.12) + 15.61 = 15.81, \tag{23}$$

and upper bound is

$$\frac{1}{\beta_{min}}(\sum_{i=1}^{5} \beta_i z_i - \prod_{i=1}^{5} z_i^{\beta_i}) + 5 \cdot R_g = \frac{1}{0.1} \cdot (3.18 - 3.12) + 15.61 = 16.21. \tag{24}$$

For explanation, we could note how the lower sombor index adjusts compared to the sombor index SO(G) with changing the weights of the edges (costs), as shown by the comparison of Equations (21) and (23). Similarly, we could note that how the upper sombor index adjusts compared to the sombor index SO(G) with changing the weights of the edges (costs), as shown by the comparison of Equations (22) and (24).

(ii) *Using the inequality derived from Theorem (2.9):*

We have

$$\sigma^2(\mathbf{Z}^{\frac{1}{2}}) = \frac{1}{m}\sum_{i=1}^{m} (z_i^{\frac{1}{2}} - \sum_{i=1}^{m} z_k^{\frac{1}{2}})^2 \tag{25}$$

and so,

$$\mathbf{Z}^{\frac{1}{2}} = (\sqrt{13}^{\frac{1}{2}}, \sqrt{13}^{\frac{1}{2}}, \sqrt{13}^{\frac{1}{2}}, \sqrt{5}^{\frac{1}{2}}, \sqrt{8}^{\frac{1}{2}}),$$

$$\frac{1}{5}\sum_{k=1}^{5} z_k^{\frac{1}{2}} = \frac{1}{5}(\sqrt{13}^{\frac{1}{2}} + \sqrt{13}^{\frac{1}{2}} + \sqrt{13}^{\frac{1}{2}} + \sqrt{5}^{\frac{1}{2}} + \sqrt{8}^{\frac{1}{2}}) = \frac{1}{5}(1.90 + 1.90 + 1.90 + 1.50 + 1.68) = 1.78.$$

Hence

$$\begin{aligned}\sigma^2(\mathbf{Z}^{\frac{1}{2}}) &= \frac{1}{5}\Big[(\sqrt{13}^{\frac{1}{2}} - 1.78)^2 \times 3 + (\sqrt{5}^{\frac{1}{2}} - 1.78)^2 + (\sqrt{8}^{\frac{1}{2}} - 1.78)^2\Big] \\ &= \frac{1}{5} \times 0.13 = 0.026.\end{aligned}$$

Now by considering Inequalities (11), $m(R_g + \sigma^2(\mathbf{Z}^{\frac{1}{2}})) \leq SO(G)$:

$$m(R_g + \sigma^2(\mathbf{Z}^{\frac{1}{2}})) = 15.61 + 0.13 = 15.74 \leq 15.88 = SO(G).$$

The result validates the inequality and shows how the variance of a transformed variable $Z^{\frac{1}{2}}$ *and other graph parameters* (R_g) *contribute to bounding* $SO(G)$

(iii) *Using the inequalities derived from Theorem (2.11):*

With considering

$$\sigma^2(Z) = \frac{1}{m}\sum_{i=1}^{m}(z_i - \frac{1}{m}\sum_{k=1}^{m} z_k)^2,$$

we have

$$\mu = \frac{1}{m}\sum_{k=1}^{5} z_k$$

and thus

$$\mu = \frac{1}{5}(\sqrt{13}\times 3 + \sqrt{8} + \sqrt{5}) = 3.18.$$

This means

$$\sigma^2(Z) = \frac{1}{5}\Big[(\sqrt{13}-3.18)^2\times 3 + (\sqrt{8}-3.18)^2 + (\sqrt{5}-3.18)^2\Big] = 0.31,$$

and in result by Inequalities (12), $m(R_g + \frac{\sigma^2(Z)}{2M_2}) \le SO(G) \le m(R_g + \frac{\sigma^2(Z)}{2M_1})$:

$$5(3.12 + \frac{0.31}{2\times\sqrt{13}}) \le SO(G) \le 5(3.12 + \frac{0.31}{2\times\sqrt{5}})$$
$$\Rightarrow 15.81 \le SO(G) \le 15.96.$$

(iv) *Using the inequalities derived from Theorem (2.14):*

$$\sigma = \sqrt{\sigma^2} = \sqrt{0.31} = 0.56,$$

so by inequalities (13), $\frac{m}{\sqrt{m-1}}\sigma < SO(G) \le m(R_g + \sqrt{m-1}\,\sigma)$:

$$\frac{5}{2}\times 0.56 \le SO(G) \le 5(3.12 + 2\times 0.56).$$

Thus

$$1.4 \le SO(G) \le 21.2.$$

Example 3.2. *Let* $G(n,p)$ *be a random graph with* $n = 5$ *vertices and* $m = 5$ *edges. If the degree-radii follow a binomial distribution with probability* $p = \frac{1}{2}$, *and*

$$R_g = 3.12, \quad M_1 = \sqrt{5} \quad \text{and} \quad M_2 = \sqrt{13},$$

then find the lower and upper bounds for the Sombor index.

For a graph G with binomial distribution, the variance of degree-radii is given by $\sigma^2(Z) = np(1-p)$. *If each edge is selected with probability* $p = \frac{1}{2}$, *so by inequalities (12) of Theorem (2.11), we have the lower bound*

$$m(R_g + \frac{\sigma^2(Z)}{2M_2}) = 5(3.12 + \frac{5\times\frac{1}{2}(1-\frac{1}{2})}{2\times\sqrt{13}}) = 16.47$$

and the upper bound

$$m(R_g + \frac{\sigma^2(Z)}{2M_1}) = 5(3.12 + \frac{5 \times \frac{1}{2}(1 - \frac{1}{2})}{2 \times \sqrt{5}}) = 17.00.$$

So,

$$16.47 \leq SO(G) \leq 17.00.$$

Example 3.3. *Consider the graph G with*

$$z_1 = z_2 = z_3 = \sqrt{13},\ z_4 = \sqrt{8},\ z_5 = \sqrt{5}.$$

Then using Inequality (11), survey the bounds for $SO(G)$ by increasing r.

If $r = 1$, $SO(G) = 5(\frac{1}{5}(3 \times \sqrt{13} + \sqrt{8} + \sqrt{5})) = 15.88$.

If $r = 2$, $SO(G) \leq 5 \times (\frac{1}{5}\sum_{i=1}^{5} z_i^2)^{\frac{1}{2}}$ then $SO(G) \leq 5 \times (\frac{1}{5}(3 \times 13 + 8 + 5))^{\frac{1}{2}} = 16.12$.

If $r = 3$, $SO(G) \leq 5 \times (\frac{1}{5}\sum_{i=1}^{5} z_i^3)^{\frac{1}{3}}$ then $SO(G) \leq 5 \times (\frac{1}{5}(3 \times \sqrt{13}^3 + \sqrt{8}^3 + \sqrt{5}^3))^{\frac{1}{3}} = 16.34$.

If $r = 4$, $SO(G) \leq 5 \times (\frac{1}{5}\sum_{i=1}^{5} z_i^4)^{\frac{1}{4}}$ then $SO(G) \leq 5 \times (\frac{1}{5}(3 \times 13^2 + 8^2 + 5^2)^{\frac{1}{4}} = 16.52$.

$\vdots$

If $r \to \infty$, $SO(G) \leq \lim_{r\to\infty} 5 \times (\frac{1}{5}\sum_{i=1}^{5} z_i^r)^{\frac{1}{r}}$ then $SO(G) \leq \lim_{r\to\infty} 5 \times (\frac{1}{5}(\sqrt{13}^r)^{\frac{1}{r}} = 5\sqrt{13} = 18.03$

As you consider, the upper bound increases as we use higher values of r. In fact, the tighter bounds are obtained from the lower-order means, and as r increases, the bounds become looser.

Example 3.4. *Consider graph G with*

$$z_1 = z_2 = z_3 = \sqrt{13},\ z_4 = \sqrt{8},\ z_5 = \sqrt{5}.$$

Calculate $SO(G)$, SO_{st}, SO_μ.

For this graph, we obtain $\sigma = 0.56$, $\mu = 3.18$, and $SO(G) = 15.88$.

Now based on the definition $SO_{st}(G)$ in Theorem (2.4) we compute $x_i = \frac{z_i - \mu}{\sigma}$, which gives

$$z_1 = z_2 = z_3 = 0.76,\ z_4 = -0.63,\ z_5 = -1.69 \Rightarrow SO_{st} = -0.04.$$

Based on the definition $SO_\mu(G)$ in Theorem (2.25), we have

$$SO_\mu(G) = 3|\sqrt{13} - 3.18| + |\sqrt{8} - 3.18| + |\sqrt{5} - 3.18| = 2.57.$$

4 Conclusion

In this paper, we provide some tight and loos bounds for the Sombor index using topological and probebilistic methods. Additionally, a bound for comparing the Sombor index of weighted graphs is introduced, using weights from a unit fraction.

Furthermore, we examine the ratio

$$\frac{m.R_g}{SO(G)},$$

in regular graphs and Erdös-Rényi random graphs, and prove that in regular graphs this value equals one, while in Erdös-Rényi random graphs, as m tends to infinity, this value approaches $e^{-\gamma}$. This enables us to uncover certain structural and molecular properties of chemical graphs and predict some of them.

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Data Availability

The data used to support the findings of this study are included within the article.

Conflicts of Interest

The authors declare that they have no conflicts of interest regarding the publication of this article.

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