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Euler-Sombor index and its congeners

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Abstract: The Euler-Sombor index EU is a vertex-degree-based graph invariant, defined as the sum over all pairs of adjacent vertices u, v of the underlying graph, of the terms $\sqrt{d_u^2 + d_v^2 + d_u\, d_v}$, where d_u and d_v are the degrees of the vertices u and v, respectively. For a real number λ, a variable version of EU is constructed, denoted by $EU(\lambda)$, defined via $\sqrt{d_u^2 + d_v^2 + \lambda\, d_u\, d_v}$. Its special cases for $\lambda = 2, -2, 0$, and 1 are, respectively, the first Zagreb, Albertson, Sombor, and the ordinary Euler-Sombor indices. The basic properties of $EU(\lambda)$ are determined, including a method for its approximate calculation and bounds in terms of minimum degree, maximum degree, order and size for several graph products. It is shown how to find values of λ for which $EU(\lambda)$ is optimal with regard to predicting molecular properties.

Keywords: degree (of vertex), vertex-degree-based graph invariant, Sombor index, Euler-Sombor index

MSC: 05C07, 05C09.

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1. Introduction

The Sombor index SO is a recently discovered vertex-degree-based graph invariant [1,2], defined as

$$SO = SO(G) = \sum_{uv \in \mathbf{E}(G)} \sqrt{d_u^2 + d_v^2}\,. \tag{1}$$

Initially, it was aimed at solving chemical problems [3] but in the meantime it found peculiar applications is various other fields of science and technology, see e.g. [4–7]. The mathematical properties of $SO(G)$ are nowadays studied in due detail [8]. In [9] an elliptic geometric model for Sombor-type indices was proposed. Within this model, the perimeter of the considered ellipse could be (approximately) calculated by means of Euler's formula [10] $\pi\, \sqrt{2(r_1 + r_2)}$, where r_1 and r_2 are the semi-major and semi-minor axes of the ellipse. In [9] it was shown that

$$r_1 = \sqrt{d_u^2 + d_v^2} \qquad \text{and} \qquad r_2 = \frac{1}{\sqrt{2}}\,(d_u + d_v),$$

which implies that the perimeter is $\sqrt{3}\pi\, \sqrt{d_u^2 + d_v^2 + \frac{2}{3}\, d_u\, d_v}$. This was the motivation to introduce a new Sombor-type graph invariant [11], defined as

$$EU = EU(G) = \sum_{uv \in \mathbf{E}(G)} \sqrt{d_u^2 + d_v^2 + d_u\, d_v}, \tag{2}$$

and named Euler-Sombor index, see also [12–14].

In the present paper we examine a variable version of the Euler-Sombor index, defined as

$$EU(\lambda) = EU(\lambda, G) = \sum_{uv \in \mathbf{E}(G)} \sqrt{d_u^2 + d_v^2 + \lambda\, d_u\, d_v}, \tag{3}$$

where λ is a real number.

In the above formulas, G stands for a simple graph with vertex set $\mathbf{V}(G)$ and edge set $\mathbf{E}(G)$. If the vertices $u,v \in \mathbf{V}(G)$ are adjacent, then the edge connecting them is denoted by uv. The degree of a vertex $u \in \mathbf{V}(G)$ is denoted by d_u. The summations in the above formulas go over all edges uv of the underlying graph G. For other graph-theoretical notation and terminology, we refer to [15,16]. For details of chemical graph theory, especially for applications of topological indices see [17,18].

Today, in the mathematical and chemical literature there is a legion of vertex-degree-based graph invariants [19–22]. Of these, for the present considerations we need the following two.

The oldest vertex-degree-based molecular structure descriptor is the first Zagreb index, [23], defined as

$$M_1 = M_1(G) = \sum_{uv \in \mathbf{E}(G)} \left[d_u + d_v\right] . \tag{4}$$

The oldest graph-theoretical irregularity measure is the Albertson index [24]

$$Alb = Alb(G) = \sum_{uv \in \mathbf{E}(G)} \left|d_u - d_v\right| . \tag{5}$$

For details on the first Zagreb and Albertson irregularity indices see [25,26] and [27,28], respectively.

At the first glance, formulas (1)–(5) appear to have quite different algebraic forms. Yet, they may be related using the following results that are obtained by direct calculation, taking into account Eqs. (1)–(5).

Proposition 1. *Let λ be a real number and let $EU(\lambda, G)$ be the corresponding variable Euler-Sombor index. Then*

$$\begin{aligned}
EU(2,G) &= M_1(G), && (6)\\
EU(-2,G) &= Alb(G), && (7)\\
EU(0,G) &= SO(G), && (8)\\
EU(1,G) &= EU(G). && (9)
\end{aligned}$$

Equalities (6)–(9) hold for any (simple) graph G.

The relations stated in Proposition 1 may be considered as the basic mathematical property of the variable Euler-Sombor index.

Proposition 2. *In the general case, $EU(\lambda)$ is well-defined (i.e., real-valued) only for $\lambda \geq -2$.*

Proof. In formula (3), the term $d_u^2 + d_v^2 + \lambda\, d_u\, d_v$ must always be positive-valued or zero. Noting that $d_u^2 + d_v^2 + \lambda\, d_u\, d_v = (d_u - d_v)^2 + (\lambda + 2) d_u\, d_v$, and that in some graphs the case $d_u = d_v$ may happen, we see that it must be $\lambda + 2 \geq 0$. $\square$

2. An approximation for variable Euler-Sombor index

Although for some chosen value of the variable λ, the actual value of the function $EU(\lambda)$ can be directly calculated by means of Eq. (3), a much easier way to do this would be by using the relations (6)–(9). Because the properties of the first Zagreb, Albertson irregularity, and Sombor indices are best understood and most detailed investigated, see [25,26], [27,28], and [8], respectively, we use the formulas (6)–(8) to obtain a second-degree polynomial approximation. By setting

$$EU(\lambda) \approx a\,\lambda^2 + b\,\lambda + c,$$

and adjusting that for $\lambda = -2, 0$, and +2, $a\,\lambda^2 + b\,\lambda + c$ be equal to Alb, SO, and M_1, respectively, we obtain

$$\begin{aligned}
a &= \frac{1}{8}(M_1 + Alb - 2\,SO),\\
b &= \frac{1}{4}(M_1 - Alb),
\end{aligned}$$

$$c = SO,$$

i.e.,

$$EU(\lambda) \approx \frac{\lambda^2}{8}(M_1 + Alb - 2\,SO) + \frac{\lambda}{4}(M_1 - Alb) + SO. \tag{10}$$

The approximation (10) is best applicable for $\lambda \in [-2, +2]$. Its quality is seen from Figure 1.

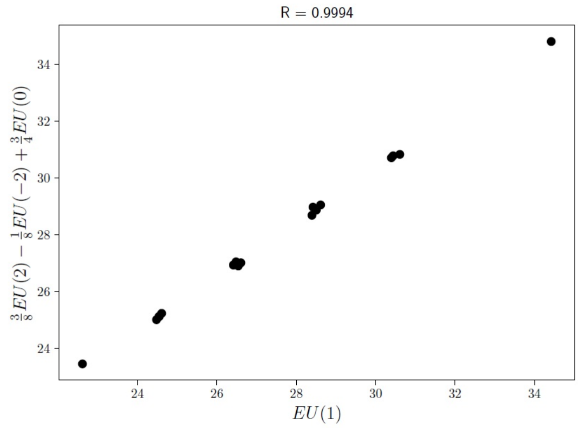

Figure 1. The Euler-Sombor index ($EU(\lambda)$ for $\lambda = 1$) calculated by means of formula (10), for the set of isomeric octanes; R is the correlation coefficient

3. Variable Euler-Sombor index of graph products

In this section, we assume that the graphs considered are simple, finite, undirected and connected. For details on graph products see [29].

3.1. Corona product

The corona product of graphs G and H is the graph denoted by $G \bigodot H$, obtained by taking one copy of G and n_G copies of H, and joining the vertex u that is on i-th position in G to every vertex in i-th copy of H. The order and size of $G \bigodot H$ are $n_G(1 + n_H)$ and $m_G + n_G m_H + n_G n_H$, respectively.

The degree of a vertex $u \in \mathbf{V}(G \bigodot H)$ is given by

$$d_{G \bigodot H}(u) = \begin{cases} d_G(u) + n_H, & if\, u \in \mathbf{V}(G), \\ d_H(u) + 1, & if\, u \in \mathbf{V}(H). \end{cases} \tag{11}$$

Theorem 1. *Let G and H be graphs with maximum degrees $\Delta_G\, \Delta_H$ and minimum degrees δ_G, δ_H, respectively. Then, $\mu_1 \le EU(\lambda, G \bigodot H) \le \mu_2$, where*

$$\mu_1 = m_G\sqrt{\lambda+2}(\delta_G + n_H) + m_H\sqrt{\lambda+2}(\delta_H + 1) + n_G\, n_H\sqrt{\lambda(\delta_G + n_H)(\delta_H + 1)},$$

and

$$\mu_2 = m_G\sqrt{\lambda+2}(\Delta_G + n_H) + m_H\sqrt{\lambda+2}(\Delta_H + 1) + n_G\, n_H\sqrt{\lambda(\Delta_G + n_H)(\Delta_H + 1)}\,.$$

Equality holds if and only if G and H are regular graphs.

Proof. By using the definitions of variable Euler-Sombor index and (11), we obtain

$$EU(\lambda, G \bigodot H) = \sum_{uv \in \mathbf{E}(G)} \sqrt{(d_G(u) + n_H)^2 + (d_G(v) + n_H)^2 + \lambda(d_G(u) + n_H)(d_G(v) + n_H)}$$

$$
\begin{aligned}
&+n_G \sum_{uv\in \mathbf{E}(H)} \sqrt{(d_H(u)+1)^2+(d_H(v)+1)^2+\lambda(d_H(u)+1)(d_H(v)+1)} \\
&+\sum_{u\in \mathbf{V}(G)} \sum_{u\in \mathbf{V}(H)} \sqrt{(d_G(u)+n_H)^2+(d_G(v)+1)^2+\lambda(d_G(u)+n_H)(d_G(v)+1)} \\
\leq\ & m_G\sqrt{\lambda+2}\,(\Delta_G+n_H)+m_H\sqrt{\lambda+2}\,(\Delta_H+1)+n_G\, n_H\sqrt{\lambda(\Delta_G+n_H)(\Delta_H+1)}\,.
\end{aligned}
$$

The lower bound is obtained in an analogous manner. □

3.2. Cartesian product

The Cartesian product of G and H is the graph denoted by $G \times H$, with vertex set $\mathbf{V}(G) \times \mathbf{V}(H)$ and two vertices $u = (u_1, v_1)$ and $v = (u_2, v_2)$ being adjacent in $G \times H$ whenever $u_1 = u_2$ and v_1 and v_2 are adjacent in H or $v_1 = v_2$ and u_1 and u_2 are adjacent in G. The size of the Cartesian product of the graphs G and H is $m_G n_H + n_G m_H$.

The degree of a vertex $(u, v) \in \mathbf{V}(G \times H)$ is

$$d_{G\times H}(u,v) = d_G(u) + d_H(v)\,. \tag{12}$$

Theorem 2. *Let G and H be graphs with maximum degrees Δ_G,Δ_H and minimum degrees δ_G,δ_H, respectively. Then,*

$$\sqrt{\lambda+2}(\delta_G+\delta_H)m_{G\times H} \leq EU(\lambda, G\times H) \leq \sqrt{\lambda+2}(\Delta_G+\Delta_H)m_{G\times H}\,.$$

Equality on both sides holds if and only if G and H are regular graphs.

Proof. By using the definitions of variable Sombor-Euler index and (12), and setting

$$X_1 = (d_G(u_1)+d_H(v_1))^2 + (d_G(u_1)+d_H(v_2))^2 + \lambda(d_G(u_1)+d_H(v_1))(d_G(u_1)+d_H(v_2)),$$

and

$$X_2 = (d_G(u_1)+d_H(v_1))^2 + (d_G(u_2)+d_H(v_1))^2 + \lambda(d_G(u_1)+d_H(v_1))(d_G(u_2)+d_H(v_1)),$$

we obtain

$$
\begin{aligned}
EU(\lambda, G\times H) &= \sum_{u_1\in \mathbf{V}(G)} \sum_{v_1v_2\in E(H)} \sqrt{X_1} + \sum_{v_1\in \mathbf{V}(G)} \sum_{u_1u_2\in \mathbf{E}(G)} \sqrt{X_2} \\
&\leq \sqrt{\lambda+2}(\Delta_G+\Delta_H)(m_G\, n_H + n_G\, m_H) \\
&= \sqrt{\lambda+2}(\Delta_G+\Delta_H)m_{G\times H}\,.
\end{aligned}
$$

The lower bound is obtained in an analogous manner. □

3.3. Lexicographic product

The lexicographic product of G and H is the graph denoted by $G[H]$, whose vertex set is $\mathbf{V}(G) \times \mathbf{V}(H)$, and two vertices $u = (u_1, u_2)$ and $v = (v_1, v_2)$ are adjacent in $G[H]$ whenever $u_1v_1 \in \mathbf{E}(G)$ or $u_1 = v_1$ and $u_2v_2 \in \mathbf{E}(H)$. The size of $G[H]$ is $m_G\, n_H^2 + n_G\, m_H$.

The degree of a vertex $(u, v) \in \mathbf{V}(G[H])$ is

$$d_{G[H]}(u,v) = n_H d_G(u) + d_H(v)\,. \tag{13}$$

Theorem 3. *Let G and H be graphs with maximum degrees Δ_G, Δ_H and minimum degrees δ_G, δ_H, respectively. Then,*

$$\sqrt{\lambda+2}(n_H\delta_G+\delta_H)m_{G[H]} \leq EU(\lambda, G[H]) \leq \sqrt{\lambda+2}(n_H\Delta_G+\Delta_H)m_{G[H]}\,.$$

The equality on both sides holds if and only if G and H are regular graphs.

Proof. By using the definitions of variable Euler-Sombor index and (13), and setting

$$Y_1 = (n_H\, d_G(u_1) + d_H(v_1))^2 + (n_H\, d_G(u_1) + d_H(v_2))^2 + \lambda(n_H\, d_G(u_1) + d_H(v_1))(n_H\, d_G(u_1) + d_H(v_2)),$$

and

$$Y_2 = (n_H d_G(u_1) + d_H(v_1))^2 + (n_H d_G(u_2) + d_H(v_2))^2 + \lambda(n_H d_G(u_1) + d_H(v_1))(n_H d_G(u_2) + d_H(v_2)),$$

we obtain

$$\begin{aligned} EU(\lambda, G[H]) &= \sum_{u_1\in \mathbf{V}(G)} \sum_{v_1v_2\in \mathbf{E}(H)} \sqrt{Y_1} + \sum_{v_1\in \mathbf{V}(H)} \sum_{v_2\in \mathbf{V}(H)} \sum_{u_1u_2\in \mathbf{E}(G)} \sqrt{Y_2} \\ &\le \sqrt{\lambda+2}(n_H\,\Delta_G + \Delta_H)(m_G\, n_H^2 + n_G\, m_H) \\ &= \sqrt{\lambda+2}(n_H\,\Delta_G + \Delta_H) m_{G[H]}\,. \end{aligned}$$

□

3.4. Strong product

The strong product of G and H is the graph denoted by $G \boxtimes H$, whose vertex set is $\mathbf{V}(G) \times \mathbf{V}(H)$, and two vertices $u = (u_1, u_2)$ and $v = (v_1, v_2)$ are adjacent in $G \boxtimes H$ whenever $u_1 = u_2$ and v_1 and v_2 are adjacent in H or $v_1 = v_2$ and or u_1 and u_2 are adjacent in G or u_1 and u_2 are adjacent in G and v_1 and v_2 are adjacent in H.

The degree of a vertex $(u, v) \in V(G \boxtimes H)$ is

$$d_{G\boxtimes H}(u, v) = d_G(u) + d_H(v) + d_G(u)\, d_H(v)\,. \tag{14}$$

Theorem 4. *Let G and H be graphs with maximum degrees Δ_G, Δ_H and minimum degrees δ_G, δ_H, respectively. Then,*

$$\sqrt{\lambda+2}(\delta_G + \delta_H + (\delta_G\,\delta_H)) m_{G\boxtimes H} \le EU(\lambda, G \boxtimes H) \le \sqrt{\lambda+2}(\Delta_G + \Delta_H + (\Delta_G\,\Delta_H)) m_{G\boxtimes H}\,.$$

The equality on both sides holds if and only if G and H are regular graphs.

Proof. By taking

$$\begin{aligned} A &= (d_G(u_1) + d_H(v_1) + d_G(u_1)\, d_H(v_1))^2, \\ B &= (d_G(u_1) + d_H(v_2) + d_G(u_1)\, d_H(v_2))^2, \\ C &= (d_G(u_2) + d_H(v_1) + d_G(u_2)\, d_H(v_1))^2, \end{aligned}$$

and using Eq. (14), we get

$$\begin{aligned} EU(\lambda, G\boxtimes H) &= \sum_{u_1\in \mathbf{V}(G)} \sum_{v_1v_2\in E(H)} \sqrt{A + B + \lambda(AB)} + \sum_{v_1\in \mathbf{V}(H)} \sum_{u_1u_2\in \mathbf{E}(G)} \sqrt{A + C + \lambda(AC)} \\ &\quad + 2 \sum_{u_1u_2\in \mathbf{E}(G)} \sum_{v_1v_2\in \mathbf{E}(H)} \sqrt{A + D + \lambda(AD)} \\ &\le \sqrt{\lambda+2}(\Delta_G + \Delta_H + (\Delta_G\,\Delta_H))(n_G\, m_H + m_G\, n_H + 2m_G\, m_H) \\ &= \sqrt{\lambda+2}(\Delta_G + \Delta_H + (\Delta_G\,\Delta_H)) m_G \boxtimes H. \end{aligned}$$

The lower bound is obtained analogously. □

4. Towards chemical applications of $EU(\lambda)$

Within this section, we consider as an example the standard entropy S^0 of the set of 18 isomeric octanes. What immediately comes to the mind is that by using values of λ, different from -2,0,1,2, we may improve the correlation between S^0 and $EU(\lambda)$. This would mean that the structure-dependence of S^0 is modeled by means of some (not necessarily linear) combination of topological indices M_1, SO, EU, and Alb. Unfortunately, as seen from Figure 2, this simple approach is not successful (at least in the case of entropy, at least in the case of octane isomers).

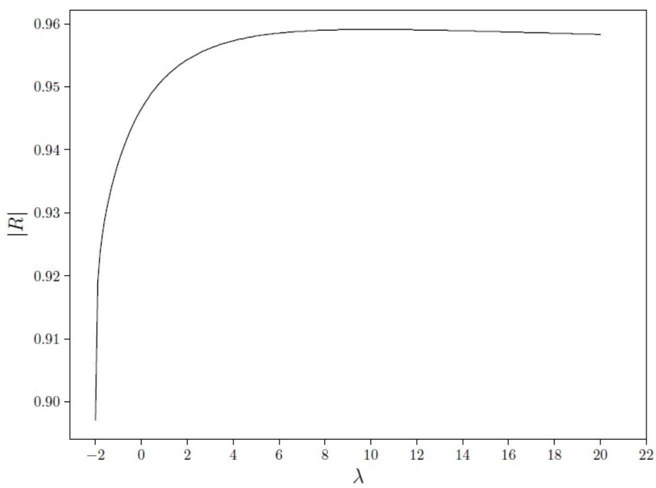

Figure 2. The λ-dependence of the correlation coefficient R for the correlation between standard entropy of octane isomers and the variable Euler-Sombor index $EU(\lambda)$. No maximum is envisaged

Bearing this difficulty in mind, a multilinear correlation between S^0 and $EU(\lambda)$ would be necessary to consider. Its general form would be $EU(\lambda) + \alpha\, EU(\mu)$, with variable λ, μ, and α.

Our preliminary testing indicates that the "optimal" values for the parameters λ, μ, and α depend very much on the physico-chemical quantity considered, and on the data set used. Therefore, in what follows we only present two characteristic examples.

Example 1. As a first guess, we choose $\mu = -\lambda$ and, to simplify, set $\alpha = 1$. The results thus obtained are shown in Figure 3.

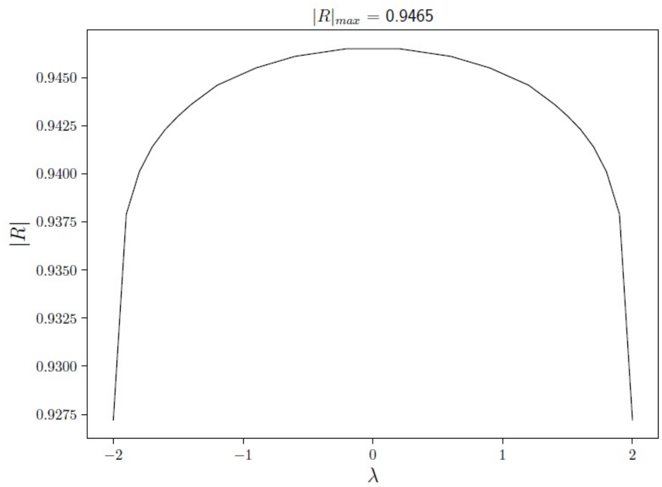

Figure 3. The λ-dependence of the correlation coefficient R for the correlation between standard entropy of octanes and $EU(\lambda) + EU(-\lambda)$. The maximum is at $\lambda = 0$, implying that for this model the best correlation is obtained with the Sombor index

Example 2. The curve depicted in Figure 3 is symmetric with regard to $\lambda = 0$ because the underlying model was chosen to be symmetric. In order to eliminate such symmetry, we now consider the model $\mu = -\lambda$ and $\alpha = 1/2$, see Figure 4.

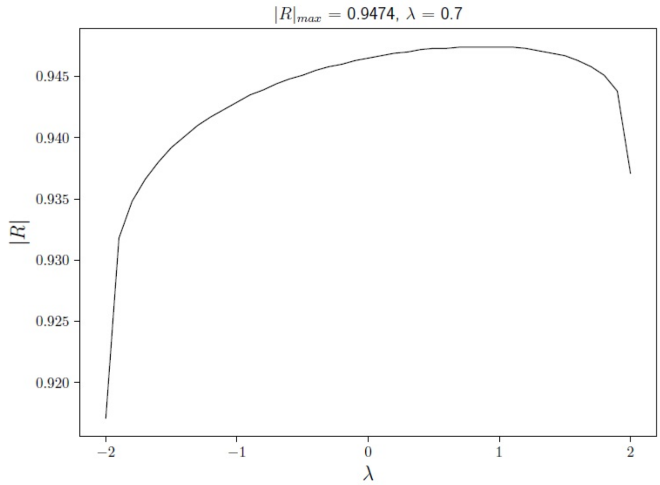

Figure 4. The λ-dependence of the correlation coefficient R for the correlation between standard entropy of octanes and $EU(\lambda) + (1/2)\,EU(-\lambda)$. The maximum is at $\lambda = 0.7$

In view of Eq. (10), the model $EU(\lambda) + (1/2)\,EU(-\lambda)$ yields optimal results at the following peculiar combinations of topological indices:

$$\begin{aligned} S^0 &\approx \frac{3 \cdot 0.7^2}{16}(M_1 + Alb + 2\,SO) + \frac{0.7}{8}(M_1 - Alb) + \frac{3}{2}\,SO \\ &= 70.179375\,M_1 - 0.004375\,Alb + 1.315250\,SO\,. \end{aligned}$$

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Data Availability: No data is required for this research.

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