On the KG-Sombor index

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Abstract:

Introduction/purpose: Degree-based graph invariants are a type of molecular descriptor that represent the connectivity of atoms (vertices) in a molecule through bonds (edges). They are used to model structural properties of molecules and provide valuable information for fields such as physical chemistry, pharmacology, environmental science, and material science. Recently, novel degree-based molecular structure descriptors, known as Sombor index-like graph invariants, have been explored from a geometrical perspective. These graph invariants have found applications in network science, where they are used to model dynamic effects in biological, social, and technological complex systems. There is also emerging interest in their potential military applications. Among these descriptors is the KG-Sombor index which is defined using both vertex and edge degrees.

Methods: The study uses combinatorial graph theory to identify and analyze extremal graphs that either maximize or minimize the KG-Sombor index.

Results: The extremal graphs are characterized concerning the KG-Sombor index, with a particular focus on trees, molecular trees, and unicyclic graphs.

Conclusion: This research advances the theoretical understanding of Sombor index-like graph invariants.

Key words: KG-Sombor index, tree, unicyclic graph, molecular tree.

Introduction

Let $G = (V, E)$ be a graph with the vertex set V and the edge set E. For a vertex v, the degree of the vertex v, denoted by d_v, is the number of edges incident with v. The first Zagreb index M_1 and the second Zagreb index M_2 of the graph G are among the most famous and extensively studied vertex-degree-based topological indices (Gutman & Das, 2004; Horoldagva et al., 2021; Selenge & Horoldagva, 2015; Zhang & Zhang, 2006) defined as:

$$M_1(G) = \sum_{uv\in E}(d_u + d_v) \quad \text{and} \quad M_2(G) = \sum_{uv\in E} d_u d_v.$$

For an edge uv, (d_u, d_v) and (d_v, d_u) are referred to as the degree-points of the edge uv. Let O be the origin of the coordinate system, and $M(d_u, d_v)$ and $M^*(d_v, d_u)$ represent the degree-points of an edge. The distance between the points O and M is $\sqrt{d_u^2 + d_v^2}$. Computing this for all edges in a graph and summing them yields the Sombor index (Gutman, 2021), defined as:

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

The Sombor-type indices (Dorjsembe & Horoldagva, 2022; Gutman, 2022, 2024; Tang et al., 2023) represent the latest addition to a plethora of topological indices in chemistry. The degree of an edge $e = uv \in E$, denoted by d_e, is the number of edges incident to e. In (Kulli et al., 2022); a novel topological graph invariant named the KG-Sombor index is introduced:

$$KG(G) = \sum_{ue} \sqrt{d_u^2 + d_e^2}, \qquad (2)$$

where $\sum_{ue}$ denotes summation over the vertices $u \in V$ and the edges $e \in E$ incident to u. Some fundamental properties of the KG-Sombor index are established in (Kulli et al., 2022), along with its relationships with other topological indices.

Cruz et al. (Cruz et al., 2021) and Cruz and Rada (Cruz & Rada, 2021) investigated the extremal values of the Sombor index for chemical graphs, unicyclic graphs, and bicyclic graphs. Recent studies on the Sombor index and the KG-Sombor index can be found in (Damnjanović et al., 2023; Das et al., 2021; Horoldagva & Xu, 2021; Kosari et al., 2023; Liu et al., 2022; Rada et al., 2021; Selenge & Horoldagva, 2024) and the references cited therein. In this paper, we aim to determine the extremal graphs concerning the KG-Sombor index for trees, unicyclic graphs, and chemical trees of a given order.

KG-Sombor index of trees and unicyclic graphs

For $e = uv$ of a graph G, let us denote

$$f(d_u, d_v) = \sqrt{d_u^2 + (d_u + d_v - 2)^2} + \sqrt{d_v^2 + (d_u + d_v - 2)^2} \qquad (3)$$

and call it the weight of uv. On the other hand for an edge $e = uv$, there are two terms in the summation $\sum_{ue}$. Hence, we can reformulate the KG-Sombor index as follows.

$$KG(G) = \sum_{uv \in E} f(d_u, d_v). \qquad (4)$$

Lemma 1. (Gutman & Das, 2004) Let T be a tree of order $n \geq 2$. Then $M_1(T) \geq 4n - 6$ with equality if and only if T is isomorphic to P_n.

Kulli et al. (Kulli et al., 2022) stated the following theorem without proof and mentioned that the proof is analogous to the proof of Theorem 2 in (Gutman, 2021). We now give the proof of it using the well-known result of Lemma 1.

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THEOREM 1. *Let T be a tree of order $n \geq 3$. Then*

$$4\sqrt{2}(n-3) + 2\sqrt{2} + 2\sqrt{5} \leq KG(T) \leq (n-1)(\sqrt{n^2-4n+5} + \sqrt{2n^2-6n+5}) \quad (5)$$

with equality on the left-hand side if and only if T is isomorphic to P_n, and equality on the right-hand side if and only if T is isomorphic to S_n.

Proof. From (3), one can easily show that

$$f(d_u, d_v) \geq \frac{1}{\sqrt{2}}(d_u + d_u + d_v - 2) + \frac{1}{\sqrt{2}}(d_v + d_u + d_v - 2) = \frac{1}{\sqrt{2}}(3(d_u + d_v) - 4) \quad (6)$$

with equality if and only if $d_u = d_v = 2$.

Since T is the tree, it has at least two pendent edges. Let us denote by $f(1, d_x)$ and $f(1, d_y)$ the weights of two pendent edges e_1 and e_2, respectively. Then $d_x \geq 2$, $d_y \geq 2$ and

$$f(1, d_x) = \sqrt{1 + (d_x - 1)^2} + \sqrt{d_x^2 + (d_x - 1)^2}. \quad (7)$$

First, it is shown that for $d_x \geq 2$,

$$f(1, d_x) \geq \frac{3\sqrt{2}}{2} d_x + \sqrt{5} - 2\sqrt{2} = g(d_x) \quad (8)$$

with equality if and only if $d_x = 2$. If $2 \leq d_x \leq 6$ then from (7) and (8), one obtains $f(1,2) = \sqrt{5}+\sqrt{2} = g(2)$, $\sqrt{5}+\sqrt{13} = f(1,3) > g(3) = 2.5\sqrt{2}+\sqrt{5}$, $\sqrt{10} + 5 = f(1,4) > g(4) = 4\sqrt{2} + \sqrt{5}$, $\sqrt{17} + \sqrt{41} = f(1,5) > g(5) = 5.5\sqrt{2} + \sqrt{5}$ and $\sqrt{26} + \sqrt{61} = f(1,6) > g(6) = 7\sqrt{2} + \sqrt{5}$. On the other hand, one gets

$$f(1, d_x) > d_x - 1 + \sqrt{2}(d_x - 1) = (1 + \sqrt{2})(d_x - 1)$$

and from this it can easily be seen that inequality (8) holds for all $d_x \geq 7$.

Similarly as the above there is

$$f(1, d_y) \geq \frac{3\sqrt{2}}{2} d_y + \sqrt{5} - 2\sqrt{2} \quad (9)$$

with equality if and only if $d_y = 2$.

Then by the definition of the KG-Sombor index and (6), one gets

$$\begin{aligned}
KG(T) = \sum_{uv\in E} f(d_u,d_v) = & \sum_{uv\in E\setminus\{e_1,e_2\}} f(d_u,d_v) + f(1,d_x) + f(1,d_y) \\
\geq & \frac{1}{\sqrt{2}} \sum_{uv\in E\setminus\{e_1,e_2\}} [(3(d_u+d_v)-4)] + f(1,d_x) + f(1,d_y) \\
= & \frac{3}{\sqrt{2}} \sum_{uv\in E(T)} (d_u+d_v) + f(1,d_x) + f(1,d_y) \\
& - \frac{3}{\sqrt{2}}(d_x+d_y+2) - \frac{4}{\sqrt{2}}(n-3) \\
= & \frac{3\sqrt{2}}{2} M_1(T) + f(1,d_x) + f(1,d_y) - \frac{3\sqrt{2}}{2}(d_x+d_y+2) - 2\sqrt{2}(n-3).
\end{aligned}$$

Then, using (8), (9) and Lemma 1 in the above inequality gives the lower bound in (5). From (6), (8), (9) and Lemma 1, it can be easily concluded that the left-hand side inequality in (5) holds if and only if T is isomorphic to P_n,

To prove the right-hand side inequality, let us consider the function

$$\phi(x) = \sqrt{x^2+(n-2)^2} + \sqrt{(n-x)^2+(n-2)^2}$$

and

$$\begin{aligned}
\phi''(x) = & \frac{1}{\sqrt{x^2+(n-2)^2}} - \frac{x^2}{(x^2+(n-2)^2)^{3/2}} + \frac{1}{\sqrt{(n-x)^2+(n-2)^2}} \\
& - \frac{x^2}{((n-x)^2+(n-2)^2)^{3/2}} \\
= & (n-2)^2 \left(\frac{1}{(x^2+(n-2)^2)^{3/2}} + \frac{1}{((n-x)^2+(n-2)^2)^{3/2}} \right) > 0.
\end{aligned}$$

Therefore the function $\phi(x)$ is convex and if $1 \leq x \leq n-1$ then the maximum of ϕ is attained at $x = 1$ or $x = n-1$.

Let $uv \in E$. Then since T is a tree, one obtains

$$2(n-1) = 2|E| = \sum_{w\in V} d_w \geq d_u + d_v + n - 2$$

that is, $d_u + d_v \leq n$. Therefore,

$$f(d_u,d_v) \leq \sqrt{d_u^2+(n-2)^2} + \sqrt{d_v^2+(n-2)^2} \leq \phi(d_u) \leq \phi(1) = \phi(n-1)$$

from $\phi(x)$ is convex. Then, by the definition of the KG-Sombor index, one gets

$$KG(T) = \sum_{uv \in E} f(d_u, d_v) \leq \sum_{uv \in E} \phi(1) = (n-1)\phi(1)$$

that is our required upper bound. Suppose now that the right-hand side equality holds in (5). Then $d_u = 1$ and $d_v = n-1$ for all $uv \in E$. Hence T is a star S_n and one can see easily that the right-hand side equality holds in (5) for S_n. This completes the proof. □

LEMMA 2. (Zhang & Zhang, 2006) Let G be a unicyclic graph of order $n \geq 3$. Then $M_1(G) \geq 4n$ with equality if and only if G is isomorphic to C_n.

THEOREM 2. *Let G be a unicyclic graph of order $n \geq 3$. Then*

$$KG(G) \geq 4n\sqrt{2}$$

with equality if and only if G is isomorphic to C_n.

Proof. Let uv be an edge of G. Then, similarly as in the proof of the previous theorem, one gets

$$f(d_u, d_v) \geq \frac{1}{\sqrt{2}}(3(d_u + d_v) - 4)$$

with equality if and only if $d_u = d_v = 2$. Therefore, by the above inequality and Lemma 2, one obtains

$$\begin{aligned} KG(G) &= \sum_{uv \in E} f(d_u, d_v) \geq \frac{3}{\sqrt{2}} \sum_{uv \in E} (d_u + d_v) - 2n\sqrt{2} \\ &= \frac{3}{\sqrt{2}} M_1(G) - 2n\sqrt{2} \geq 4n\sqrt{2} \end{aligned}$$

with equality if and only if G is isomorphic to C_n. □

KG-Sombor index of molecular trees

By Theorem 1 it is evident that the path P_n has a minimal KG-value among molecular trees of order n. Therefore, this section determines the extremal graphs with the maximal KG-value among molecular trees of order n. For $n = 3k+2$, $k \geq 1$, we denote by $\mathcal{T}_n$ the set of trees of order

n such that the degree of every vertex is either one or four. For $n = 3k$, $k \geq 3$, we denote by $\mathcal{T}_n$ the set of trees of order n such that only one vertex has degree two, and its neighbors have degree four, while the remaining vertices have degree one or four. For $n = 3k + 1$, $k \geq 4$, we denote by $\mathcal{T}_n$ the set of trees of order n such that only one vertex has degree three, and its neighbors have degree four, while the remaining vertices have degree one or four.

If $n \leq 3$ then there is only one tree of order n. If $n = 4$, then there are two trees that are P_4 and S_4, thus $KG(P_4) < KG(S_4)$. Hence, we assume that $n \geq 5$. For $n = 6$, $n = 7$, $n = 10$, we have determined the graphs with the maximum KG-Sombor index by using SageMath.

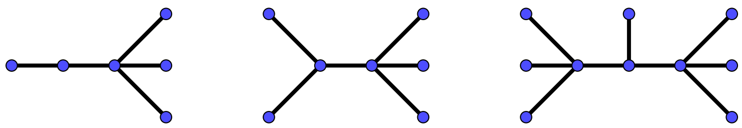

Figure 1 – Graphs with the maximum KG-Sombor index for $n = 6, 7, 10$.

The values of the KG-Sombor index of the above graphs are $3\sqrt{10} + 3\sqrt{5} + 5\sqrt{2} + 15$, $\sqrt{41} + \sqrt{34} + 2\sqrt{13} + 3\sqrt{10} + 2\sqrt{5} + 15$ and $2\sqrt{41} + 2\sqrt{34} + \sqrt{13} + 6\sqrt{10} + \sqrt{5} + 30$, respectively. For the remaining values of n, the following theorem holds.

THEOREM 3. *Let T be a molecular tree of order n.*

(i) *If $n = 3k + 2$, $k \geq 1$ then*

$$KG(T) \leq \frac{10 + 2\sqrt{10}}{3}(n + 1) + \frac{4\sqrt{13}}{3}(n - 5).$$

(ii) *If $n = 3k$, $k \geq 3$ then*

$$KG(T) \leq \frac{(10 + 2\sqrt{10})n}{3} + \frac{4\sqrt{13}n}{3} + 8\sqrt{2} + 4\sqrt{5} - 12\sqrt{13}.$$

(iii) *If $n = 3k + 1$, $k \geq 4$ then*

$$KG(T) \leq \frac{(10 + 2\sqrt{10})n}{3} + \frac{4\sqrt{13}n}{3} + 3\sqrt{34} + 3\sqrt{41} + \frac{5 + \sqrt{10}}{3} - \frac{52\sqrt{13}}{3}.$$

The equalities hold if and only if $T \in \mathcal{T}_n$*.*

Proof. Let n_i ($i = 1, 2, 3, 4$) be the number of vertices of the degree i in T. Also let $m_{i,j}$ ($1 \leq i \leq j \leq 4$) be the number of edges of T connecting the vertices of the degree i and j. Then there is $m_{1,1} = 0$ and

$$\begin{aligned}
&n_1 + n_2 + n_3 + n_4 = n\\
&m_{1,2} + m_{1,3} + m_{1,4} + m_{2,2} + m_{2,3} + m_{2,4} + m_{3,3} + m_{3,4} + m_{4,4} = n - 1\\
&m_{1,2} + m_{1,3} + m_{1,4} = n_1\\
&m_{1,2} + 2m_{2,2} + m_{2,3} + m_{2,4} = 2n_2\\
&m_{1,3} + m_{2,3} + 2m_{3,3} + m_{3,4} = 3n_3\\
&m_{1,4} + m_{2,4} + m_{3,4} + 2m_{4,4} = 4n_4.
\end{aligned} \tag{10}$$

From the above, the following equations are easily obtained:

$$\begin{aligned}
n =& \frac{3}{2}m_{1,2} + \frac{4}{3}m_{1,3} + \frac{5}{4}m_{1,4} + m_{2,2} + \frac{5}{6}m_{2,3} + \frac{3}{4}m_{2,4}\\
&+ \frac{2}{3}m_{3,3} + \frac{7}{12}m_{3,4} + \frac{1}{2}m_{4,4},\\
m_{1,4} =& \frac{2}{3}(n+1)\\
&- \frac{2}{3}\left(2m_{1,2} + \frac{5}{3}m_{1,3} + m_{2,2} + \frac{2}{3}m_{2,3} + \frac{1}{2}m_{2,4} + \frac{1}{3}m_{3,3} + \frac{1}{6}m_{3,4}\right),\\
m_{4,4} =& \frac{1}{3}(n-5) + \frac{1}{3}m_{1,2} + \frac{1}{9}m_{1,3} - \frac{1}{3}m_{2,2} - \frac{5}{9}m_{2,3} - \frac{2}{3}m_{2,4} - \frac{7}{9}m_{3,3}\\
&- \frac{8}{9}m_{3,4}.
\end{aligned} \tag{11}$$

Then, using (11), one obtains

$$\begin{aligned}
KG(T) =& \sum_{uv \in E(G)} f(d_u, d_v)\\
=& \sum_{1 \leq i \leq j \leq 4} \left[\sqrt{i^2 + (i+j-2)^2} + \sqrt{j^2 + (i+j-2)^2}\right] \cdot m_{i,j}\\
=& (\sqrt{2} + \sqrt{5})m_{1,2} + (\sqrt{5} + \sqrt{13})m_{1,3} + (5 + \sqrt{10})m_{1,4} + 4\sqrt{2}m_{2,2}\\
&+ (3\sqrt{2} + \sqrt{13})m_{2,3} + (4\sqrt{2} + 2\sqrt{5})m_{2,4} + 10m_{3,3}\\
&+ (\sqrt{34} + \sqrt{41})m_{3,4} + 4\sqrt{13}m_{4,4}\\
=& \frac{10 + 2\sqrt{10}}{3}(n+1) + \frac{4\sqrt{13}}{3}(n-5) + c_{12}m_{1,2} + c_{13}m_{1,3}
\end{aligned}$$

$$+ c_{22}m_{2,2} + c_{23}m_{2,3} + c_{24}m_{2,4} + c_{33}m_{3,3} + c_{34}m_{3,4}, \quad (12)$$

where $c_{12} = \sqrt{2} + \sqrt{5} - \frac{4(5+\sqrt{10})}{3} + \frac{4\sqrt{13}}{3} \approx -2.425$, $c_{13} = \sqrt{5} + \sqrt{13} - \frac{10(5+\sqrt{10})}{9} + \frac{4\sqrt{13}}{9} \approx -1.625$, $c_{22} = 4\sqrt{2} - \frac{2(5+\sqrt{10})}{3} - \frac{4\sqrt{13}}{3} \approx -4.592$, $c_{23} = 3\sqrt{2}+\sqrt{13} - \frac{4(5+\sqrt{10})}{9} - \frac{20\sqrt{13}}{9} \approx -3.792$, $c_{24} = 4\sqrt{2}+2\sqrt{5} - \frac{5+\sqrt{10}}{3} - \frac{8\sqrt{13}}{3} \approx -2.206$, $c_{33} = 10 - \frac{2(5+\sqrt{10})}{9} - \frac{28\sqrt{13}}{9} \approx -3.031$ and $c_{34} = \sqrt{34} + \sqrt{41} - \frac{5+\sqrt{10}}{9} - \frac{32\sqrt{13}}{9} \approx -1.492$. Note that

$$c_{22} < c_{23} < c_{33} < c_{12} < c_{13} < c_{34} < c_{24} < 0. \quad (13)$$

Now the following three cases are distinguished.

(i) If $n = 3k + 2$, $k \geq 1$ then from (12) and (13), one obtains

$$KG(T) \leq \frac{10 + 2\sqrt{10}}{3}(n + 1) + \frac{4\sqrt{13}}{3}(n - 5)$$

with equality holding if and only if

$$m_{1,2} = m_{1,3} = m_{2,2} = m_{2,3} = m_{2,4} = m_{3,3} = m_{3,4} = 0.$$

Hence one gets $n_1 = m_{1,4} = 2(n + 1)/3$ and $m_{4,4} = (n - 5)/3$. Also, there is $n_2 = n_3 = 0$.

(ii) If $n = 3k$, $k \geq 3$ then one can easily see that $n_2 \neq 0$ or $n_3 \neq 0$. If $n_2 \geq 1$ then

$$m_{1,2} + 2m_{2,2} + m_{2,3} + m_{2,4} = 2n_2 \geq 2$$

from (10). Therefore, one gets

$$\begin{aligned} KG(T) \leq& \frac{10 + 2\sqrt{10}}{3}(n + 1) + \frac{4\sqrt{13}}{3}(n - 5) \\ &+ c_{24}(m_{1,2} + 2m_{2,2} + m_{2,3} + m_{2,4}) \\ \leq& \frac{10 + 2\sqrt{10}}{3}(n + 1) + \frac{4\sqrt{13}}{3}(n - 5) + 2c_{24} \\ =& \frac{(10 + 2\sqrt{10})n}{3} + \frac{4\sqrt{13}n}{3} + 8\sqrt{2} + 4\sqrt{5} - 12\sqrt{13} \end{aligned} \quad (14)$$

since $c_{12} < c_{23} < c_{24}$ and $c_{22} < 2c_{24}$.

If $n_3 \geq 1$ then

$$m_{1,3} + m_{2,3} + 2m_{3,3} + m_{3,4} = 3n_3 \geq 3$$

from (10). Hence, one obtains

$$\begin{aligned} KG(T) \leq & \frac{10+2\sqrt{10}}{3}(n+1) + \frac{4\sqrt{13}}{3}(n-5) \\ & + c_{34}(m_{1,3} + m_{2,3} + 2m_{3,3} + m_{3,4}) \\ \leq & \frac{10+2\sqrt{10}}{3}(n+1) + \frac{4\sqrt{13}}{3}(n-5) + 3c_{34} \\ = & \frac{(10+2\sqrt{10})n}{3} + \frac{4\sqrt{13}n}{3} + 3\sqrt{34} + 3\sqrt{41} + \frac{5+\sqrt{10}}{3} \\ & - \frac{52\sqrt{13}}{3} \end{aligned} \tag{15}$$

since $c_{23} < c_{13} < c_{34}$ and $c_{33} < 2c_{34}$. From (14) and (15), one gets the required result because $3c_{34} < 2c_{24}$. Equality holds in (14) if and only if $n_2 = 1$, $n_3 = 0$ and $m_{2,4} = 2$.

(iii) If $n = 3k+1$, $k \geq 4$ then $n_2 \neq 0$ or $n_3 \neq 0$. If $n_3 \geq 1$, then similarly as in (ii), one gets

$$\begin{aligned} KG(T) \leq & \frac{(10+2\sqrt{10})n}{3} + \frac{4\sqrt{13}n}{3} + 3\sqrt{34} + 3\sqrt{41} + \frac{5+\sqrt{10}}{3} \\ & - \frac{52\sqrt{13}}{3}. \end{aligned} \tag{16}$$

Let now $n_3 = 0$. If $n_2 = 1$, then the system of equations $n_1 + n_4 = n - 1$ and $n_1 + 4n_4 = 2(n-2)$ has no integer solution. Thus $n_2 \geq 2$ and, similarly as in (ii), one also gets

$$\begin{aligned} KG(T) \leq & \frac{10+2\sqrt{10}}{3}(n+1) + \frac{4\sqrt{13}}{3}(n-5) \\ & + c_{24}(m_{1,2} + 2m_{2,2} + m_{2,3} + m_{2,4}) \\ \leq & \frac{10+2\sqrt{10}}{3}(n+1) + \frac{4\sqrt{13}}{3}(n-5) + 4c_{24} \\ < & \frac{(10+2\sqrt{10})n}{3} + \frac{4\sqrt{13}n}{3} + 3\sqrt{34} + 3\sqrt{41} + \frac{5+\sqrt{10}}{3} - \frac{52\sqrt{13}}{3} \end{aligned}$$

from $4c_{24} < 3c_{34}$. Equality holds in (16) if and only if $n_2 = 0$, $n_3 = 1$ and $m_{3,4} = 3$. On the other hand, in each case it can be easily concluded that the equality holds if and only if $T \in \mathcal{T}_n$. $\square$

Conclusions

Topological indices play a vital role in conducting quantitative structure-activity relationship and quantitative structure-property relationship studies. Numerous topological indices have been defined in the literature and several of them are applied as a means to model physical, chemical, pharmaceutical, and other properties of molecules. Gutman pioneered the introduction of SO-type indices within the field of mathematical chemistry. Our study determined the minimal and the maximal KG-Sombor index for the class of trees and chemical trees. Moreover, we proved that C_n is the unique graph with the minimal KG-Sombor index among all unicyclic graphs of order n. However, the problems of determining the graphs with the maximal KG-Sombor index in the class of unicyclic graphs, and finding the extremal KG-Sombor index in the class of bicyclic graphs remain open.

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En el índice KG-Sombor

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CAMPO: matemáticas
TIPO DE ARTÍCULO: artículo científico original

Resumen:

Introducción/objetivo: Los invariantes de gráficos basados en grados son un tipo de descriptores moleculares que representan la conectividad de los átomos (vértices) en una molécula a través de enlaces (bordes). Se utilizan para modelar propiedades estructurales de moléculas y proporcionar información valiosa para campos como la química física, la farmacología, las ciencias ambientales y las ciencias de materiales. Recientemente, se han explorado desde una perspectiva geométrica nuevos descriptores de estructuras moleculares basados en grados, conocidos como invariantes de gráficos tipo índice de Sombor. Estas invariantes gráficas han encontrado aplicaciones en la ciencia de redes, donde se utilizan para modelar efectos dinámicos en sistemas complejos biológicos, sociales y tecnológicos. También está surgiendo un interés en sus posibles aplicaciones militares. Entre estos descriptores se encuentra el índice KG-Sombor, que se define utilizando grados de vértice y borde.

Métodos: El estudio utiliza la teoría de grafos combinatoria para identificar y analizar gráficos extremos que maximizan o minimizan el índice KG-Sombor.

Resultados: Los gráficos extremos se caracterizan en relación con el índice KG-Sombor, con especial atención a árboles, árboles moleculares y gráficos unicíclicos.

Conclusión: Esta investigación avanza en la comprensión teórica de las invariantes gráficas similares al índice de Sombor.

Palabras claves: índice KG-Sombor, árbol, gráfico unicíclico, árbol molecular.

Индекс КГ-Сомбор

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РУБРИКА ГРНТИ: 27.29.19 Краевые задачи и задачи на собственные значения для обыкновенных дифференциальных уравнений и систем уравнений

ВИД СТАТЬИ: оригинальная научная статья

Резюме:

Введение/цель: Недавно с геометрической точки зрения были исследованы новые дискрипторы молекулярной структуры на основе степеней, известные как инварианты графов, подобные Сомборскому индексу. Эти инварианты графа нашли применение в сетевой науке, где они используются для моделирования динамических эффектов в биологических, социальных и сложных технологических системах. Также растет интерес к их потенциальному применению в военных целях. Среди этих дескрипторов и KG-Сомборский индекс, который определяется с использованием степеней как вершины, так и ребра.

Методы: В данном исследовании используется комбинаторная теория графов для выявления и анализа экстремальных графов, которые либо максимизируют, либо минимизируют КГ-Сомборский индекс.

Результаты: Экстремальные графы характеризуются КГ-Сомборским индексом, при этом особое внимание уделяется деревьям, молекулярным деревьям и одноциклическим графам.

Выводы: Данное исследование вносит вклад в расширение теоретического понимания инвариантов графов, подобных Сомборскому индексу.

Ключевые слова: КГ-Сомборский индекс, дерево, одноциклический граф, молекулярное дерево.

КГ-Сомборски индекс

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ОБЛАСТ: математика
КАТЕГОРИЈА (ТИП) ЧЛАНКА: оригинални научни рад

Сажетак:

Увод/циљ: На степенима засноване графовске инваријанте тип су молекуларних дескриптора који представљају повезаност атома (чворова) у молекулу путем веза (грана). Користе се за моделовање структурних својстава молекула и пружају драгоцене информације у областима попут физичке хемије, фармакологије, науке о животној средини, као и науке о материјалима. Из геометријске перспективе недавно су проучавани нови дескриптори молекуларне структуре на бази степена, познати као графовске инваријанте сродне Сомборском индексу. Ове графовске инваријанте нашле су примену у науци о мрежама где се користе за моделовање динамичких утицаја у биолошким, друштвеним и сложеним технолошким системима. Такође, постоји и интересовање за потенцијалне примене у војсци. Међу овим дескрипторима налази се КГ-Сомборски индекс који се дефинише коришћењем степенова и чворова и грана.

Методе: У истраживању се користи комбинаторна теорија графова за идентификацију и анализу екстремалних графова који или максимизују или минимизују КГ-Сомборски индекс.

Резултати: Екстремални графови се карактеришу у односу на КГ-Сомборски индекс, са посебним освртом на стабла, молекуларна стабла и уницикличне графове.

Закључак: Овим истраживањем унапређује се теоријско разумевање графовских инваријанти сродних Somборском индексу.

Кључне речи: КГ-Сомборски индекс, стабло, унициклични граф, стабло молекула.

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