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The Minimum Sombor Index for Unicyclic Graphs with Fixed Diameter

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Abstract

As a novel member of the class of vertex-degree-based topological indices, the so-called Sombor index was recently introduced by Gutman on the chemical graphs. In this paper, we present the minimum Sombor index for unicyclic graphs with the diameter $D \geq 2$.

1 Introduction

Let $G = (V, E)$ be a simple connected graph with the vertex set $V(G)$ and the edge set $E(G)$ where $|V(G)|$ is the number of vertices and $|E(G)|$ is the number of edges. The degree of a vertex $v \in V(G)$, denoted by $d_v(G)$, is the number of its neighbors and the set of all vertices adjacent to v is denoted by $N_v(G)$. A vertex of degree one is called a pendent vertex and also the edge $uv \in E(G)$ is a pendent edge of G, if $d_u = 1$ or $d_v = 1$. The graph G is the chemical graph if $d_v \leq 4$, for all $v \in V(G)$.

We denote by $d_G(u, v)$ the distance between any two distinct vertices u and v in G which is the number of edges in the shortest path travels from one of them to another. The diameter of G is defined as

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$D(G) = \{max\ d(u,v) : u, v \in V(G)\}$. A diametral path is a shortest path in G joining two vertices, say $u, v \in V(G)$, with $d_G(u,v) = D(G)$. A unicyclic graph is a connected graph G containing exactly one cycle, that is $|V(G)| = |E(G)|$. From now on, we drop the subscript "G" from the notation $d_v(G)$, $N_v(G)$ and $D(G)$ when there is no confusion.

A structural invariant to a graph is reffered to a graphical invariant. It is indicated by a numerical quantity that is invariant under graph isomorphisms. The topological index is often reserved for graphical invariant in chemical graph theory. Several types of vertex-degree-based topological indices regarded as graphical invariants have been newly introduced and extensively studied by many authors.

The ordered pair (x, y), where $x = d_u$ and $y = d_v$, is called the degree-coordinate (or d-coordinate) of the edge $uv \in E(G)$. In the coordinate system of two dimensions, it corresponds to a point called the degree-point (or d-point) of the edge uv. Based on Euclidean metric, the distance between the d-point (x, y) and the origin of the coordinate system is called the degree-radius (or d-radius) of the edge uv. This is denoted by $r(x, y)$ and defined as $r(x, y) = \sqrt{x^2 + y^2}$. From the above considation, Gutman in [5] introduced the Sombor index of a graph G given by

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

and established some basic properties of the sombor index on some molecular graphs. He determined simple lower and upper bounds for Sombor indices in [6]. It is shown that any vertex-degree-based topological index can be considered as a special case of a Sombor type index. Das et al. [3] found some relations on the Somber index with the first and second Zagreb indices. The authors presented several lower and upper bounds on the Sombor index of graphs building on some useful graph parameters such as deleting and adding edges to graph, maximum and minimum degree of vertices, and etc.

Cruz et al. [1] obtained the Sombor index of (connected) chemical graphs, chemical trees (with n vertices), and hexagonal systems (with h hexagons) as natural representations of benzenoid hydrocarbons. Deng et al. [4] investigated the chemical importance of the Sombor index. There is shown that this index is more effective in predicting physico-chemical properties with high accuracy compared to often used indices. They also obtained a sharp upper bound on the (reduced) Sombor index among all molecular trees with fixed orders, and characterized those molecular trees achieving the extremal value. Kulli and Gutman [8] proposed (reduced, modified) Sombor index of a molecular graph and computed exact formulas for certain chemical important structures such as silicate, chain silicate, oxide, and graphene networks. Redžepović [16] examined chemical applicability of Sombor indices and more precisely analyzed their predictive and discriminative potentials. He illustrated that Sombor type index showed good predictive potential. Li et al. [10] characterized the extremal graphs with respect to the Sombor index among all the n-order trees with diameter 3 and solved the corresponding extremal problem to determine the largest and the second largest Sombor indices of n-vertex trees with a given diameter greater than 4.

Kulli in [9] studied the certain Sombor indices and their corresponding polynomials of regular and complete bipartite graphs for line and subdivision graphs. Milovanović et al. [14] determined upper and lower bounds on the Sombor indices and their relationship with other degree-based indices. The authors also proved two inequalities of the Nordhaus-Gaddum type for the Sombor index.

Unicyclic graphs as one of the great classes can exhibit various chemical structures as well. Cruz et al. [2] attained minimal and maximal values of the Sombor index over unicyclic and bicyclic graphs. Réti et al. [17] derived some bounds on the Sombor index and proved that the cycle graphs C_n have the minimum Sombor index among all connected unicyclic graphs of a fixed order $n \geq 4$, and showed that the maximum Sombor index is a tool to characterize the classes of all connected unicyclic, bicyclic, tricyclic, tetracyclic, and pentacyclic graphs of a fixed order. Liu in [12] determined the maximum Sombor indices for unicyclic graphs with given diameter which is inspired by the extremal problem of trees with some parameters such as pendent vertices, diameter, matching number, segment number and branching number.

The topological indices as numerical molecular descriptors associated with the structure formulas for measuring molecular similarity or dissimilarity in structure-property and structure-activity relationship studies. Mathematical properties of these descriptors have been studied extensively. The Randić index of graphs is one of the most successful molecular descriptors, proposed by the chemist Randić [15] in 1975. Li and Shi in [11] proved two conjectures on the Randić index with relations to the diameter and the average distance of connected (molecular) graphs. Song and Pan in [18] obtained sharp lower bounds of Randić index of unicyclic graphs of a fixed order and diameter. Liu [13] found some relations between the harmonic index as a closely related variant of the Randić index and diameter of graphs. Jerline and Michaelraj in [7] solved the conjecture of Liu [13] in 2013. They presented a better bounds of the ratio of the harmonic index to the diameter on unicyclic graphs. Zhong [19] determined the minimum harmonic index for unicyclic graphs with given diameter and characterized the corresponding extremal graphs.

Now, in this paper we will attain the minimum Sombor index among all unicyclic graphs with a fixed diameter $D \geq 2$. We use the following Lemma in the proof of Theorems 1 and 2. In this Lemma, we remove one of the paths connected to a pendent vertex of G such that the desired graph G' is a subgraph of G, where its diameter is equal to diameter of G and the number of its pendent vertices is one less than G.

Lemma 1. *Let G be a unicyclic graph and suppose U be a diametral path. If G has a pendent vertex such that $v \notin V(U)$, then there exists a unicyclic graph $G' \subset G$, where $v \notin V(G^{'})$, $D(G) = D(G^{'})$ and $SO(G) > SO(G^{'})$.*

Proof. Let U be a diametral path of G and let $v \in V(G)$ be a pendent vertex such that $v \notin V(U)$. Assume that u is the nearest vertex to v with $d_u \neq 2$. Consider $G^{'} \subset G$, the graph obtained from G by removing the connecting path u to v. Let x be the neighbor of u over the connecting path u to v (if the path has only one edge, then $x = v$). It is obvious that $G^{'}$ is a unicyclic graph and $D(G^{'}) = D(G)$. Then we have

$$SO(G)-SO(G^{'}) \geq \sqrt{d_u^2+1}+\sum_{y\in N_u\setminus\{x\}}\left(\sqrt{d_u^2+d_y^2}-\sqrt{(d_u-1)^2+d_y^2}\right) > 0,$$

which implies that $SO(G) > SO(G^{'})$. ■

Lemma 2. *[17] Let G be a connected unicyclic graph with $n \geq 4$ vertices, then $SO(G) \geq SO(C_n) = n\sqrt{8}$.*

By Lemma 2, in this paper we will consider the unicyclic graphs with at least one pendent vertex.

2 Main results

In this section, we will present a lower bound on the Sombor index of the unicyclic graph with its diameter at least 3.

Theorem 1. *Let G be a unicyclic graph with n vertices and the diameter D such that $D \geq 3$ and $n \geq D + 2$. Then,*

$$SO(G) \geq SO(U_1) = (n-4)\sqrt{8} + 3\sqrt{13} + \sqrt{5},$$

where U_1 is the graph obtained from connected one path with $2D - n + 1$ edges to one vertex of the graph $C_{2n-2D-1}$.

Proof. Since G has at least one pendent vertex, therefore we consider the following three cases.

Case1: G has exactly one pendent vertex.
The graph G contains the path P with $m \geq 1$ edges and the cycle C_l with $l \geq 3$. Then C_l and P have a common vertex of degree 3 in G. Thus,

$$SO(G) = SO(C_l) + SO(P). \tag{1}$$

First let $m \geq 2$ and $l \geq 4$. The path P has one $(1,2)$-edge, one $(2,3)$-edge and $m-2$ edges of d-coordinate $(2,2)$, it follows that

$$SO(P) = (m-2)\sqrt{8} + \sqrt{13} + \sqrt{5}, \tag{2}$$

on the other hand, the cycle C_l has $l-2$ edges of d-coordinate $(2,2)$ and two $(2,3)$-edegs, hence

$$SO(C_l) = (l-2)\sqrt{8} + 2\sqrt{13}. \tag{3}$$

By substituting (2) and (3) in the formula (1) we deduce that

$$SO(G) = (m + l - 4)\sqrt{8} + 3\sqrt{13} + \sqrt{5}.$$

Since $n = l+m$, here we have $SO(G) \geq (n-4)\sqrt{8}+3\sqrt{13}+\sqrt{5} \geq SO(U_1)$. If $m = 1$ and $l \geq 4$, then $n = l + 1$ and $SO(P) = \sqrt{10}$. Therefore,

$$SO(G) = (l - 2)\sqrt{8} + 2\sqrt{13} + \sqrt{10} \geq (n - 3)\sqrt{8} + 2\sqrt{13} + \sqrt{10} \geq SO(U_1).$$

When $l = 3$ and $m \geq 2$, then $n = m + 1$ and the Sombor index has the minimum bound, $SO(G) = (n - 4)\sqrt{8} + 3\sqrt{13} + \sqrt{5} = SO(U_1)$.

Case2: The graph G has exactly two pendent vertices.
In this case, G contains two paths P and $P^{'}$ such that they have $m_1 \geq 1$ and $m_2 \geq 1$ edges, respectively. Also there exists the cycle C_l with $l \geq 3$. We can suppose that C_l and P have a common vertex and $P^{'}$ is connected either to one of the vertices of C_l or to an interior vertex of P.

Subcase 2-1: When $P \cap P^{'} = \emptyset$.
Then we have $SO(G) = SO(C_l) + SO(P) + SO(P^{'})$. First let $l \geq 4$ and $m_1, m_2 \geq 2$. Thus, any path has $m_i - 2$ edges of d-coordinate $(2, 2)$ for $i = 1, 2$, one $(1, 2)$-edge, and one $(2, 3)$-edge. It implies the following equalities $SO(P) = (m_1 - 2)\sqrt{8} + \sqrt{13} + \sqrt{5}$, and $SO(P^{'}) = (m_2 - 2)\sqrt{8} + \sqrt{13} + \sqrt{5}$. Consider P and $P^{'}$ are connected to non-adjacent vertices of C_l, therefore the cycle C_l contains four $(2, 3)$-edges and $l - 4$ edges of d-coordinate $(2, 2)$. We obtain

$$SO(C_l) = (l - 4)\sqrt{8} + 4\sqrt{13}, \tag{4}$$

and if P and $P^{'}$ are connected to adjacent vertices of C_l, then the cycle C_l has two $(2, 3)$-edges, one $(3, 3)$-edge and $l - 3$ edges of d-coordinate $(2, 2)$. Hence the following is satisfied

$$SO(C_l) = (l - 3)\sqrt{8} + 2\sqrt{13} + \sqrt{18}. \tag{5}$$

Since $n = l + m_1 + m_2$ and the relation (4) is greater than (5), we deduce the following inequalities

$$\begin{aligned}SO(G) &\geq (l+m_1+m_2-7)\sqrt{8}+4\sqrt{13}+2\sqrt{5}+\sqrt{18}\\ &\geq (n-7)\sqrt{8}+4\sqrt{13}+2\sqrt{5}+\sqrt{18} \geq (n-4)\sqrt{8}+3\sqrt{13}+\sqrt{5}.\end{aligned}$$

If $l \geq 4$ and $m_1 = 1$, $m_2 \geq 2$, then $n = l+m_2+1$ and $SO(P) = \sqrt{10}$ and also $SO(P^{'}) = (m_2-2)\sqrt{8}+\sqrt{13}+\sqrt{5}$. We have

$$\begin{aligned}SO(G) &\geq (l+m_2-5)\sqrt{8}+3\sqrt{13}+\sqrt{18}+\sqrt{10}+\sqrt{5}\\ &\geq (n-6)\sqrt{8}+3\sqrt{13}+\sqrt{18}+\sqrt{10}+\sqrt{5}\\ &\geq (n-4)\sqrt{8}+3\sqrt{13}+\sqrt{5},\end{aligned}$$

and if $l \geq 4$ and $m_1 = m_2 = 1$, then $n = l+2$ and $SO(P)+SO(P^{'}) = 2\sqrt{10}$. We conclude that

$$\begin{aligned}SO(G) &\geq (l-3)\sqrt{8}+2\sqrt{13}+2\sqrt{10}+\sqrt{18}\\ &\geq (n-5)\sqrt{8}+2\sqrt{13}+2\sqrt{10}+\sqrt{18} \geq (n-4)\sqrt{8}+3\sqrt{13}+\sqrt{5}.\end{aligned}$$

When $l = 3$ and $m_1, m_2 \geq 2$, then $n = m_1+m_2+3$ and $SO(C_l) = 2\sqrt{13}+\sqrt{18}$. It obtains that

$$\begin{aligned}SO(G) &= (m_1+m_2-4)\sqrt{8}+4\sqrt{13}+\sqrt{18}+2\sqrt{5}\\ &= (n-7)\sqrt{8}+4\sqrt{13}+\sqrt{18}+2\sqrt{5} \geq (n-4)\sqrt{8}+3\sqrt{13}+\sqrt{5}.\end{aligned}$$

If $l = 3$ and $m_1 = m_2 = 1$, then $D = 3$, $n = 5$. We have

$$SO(G) = 2\sqrt{13}+2\sqrt{10}+\sqrt{18} > \sqrt{8}+3\sqrt{13}+\sqrt{5} = (n-4)\sqrt{8}+3\sqrt{13}+\sqrt{5}.$$

Finally, when $l = 3$ and $m_1 = 1$, $m_2 \geq 2$, then $n = m_2+4$. Therefore it is proved that

$$\begin{aligned}SO(G) &\geq (m_2-2)\sqrt{8}+\sqrt{5}+\sqrt{10}+3\sqrt{13}+\sqrt{18}\\ &= (n-6)\sqrt{8}+3\sqrt{13}+\sqrt{5} \geq (n-4)\sqrt{8}+3\sqrt{13}+\sqrt{5}.\end{aligned}$$

Subcase 2-2: Assume that $P \cap P^{'} \neq \emptyset$ and there exists a diametral path U containing both pendent vertices of the graph G.

In this case, U is a subset of $P \cup P^{'}$. If both paths are connected to a vertex of C_l, then one of the interior vertices of U, say u, is of degree 4 in G and whenever path $P^{'}$ attached to one of the interior vertices of P, then one of the interior vertices of U, say u, is of degree 3 in G.

If u is not connected to a pendent vertex of U, then following inequalities hold $SO(U) \geq (D-4)\sqrt{8} + 2\sqrt{5} + 2\sqrt{13}$ or $SO(U) \geq (D-4)\sqrt{8} + 2\sqrt{5} + 2\sqrt{20}$.

Therefore we can consider the smaller value for the lower bound on the Sombor index of G such that

$$SO(U) \geq (D-4)\sqrt{8} + 2\sqrt{5} + 2\sqrt{13}. \tag{6}$$

Let u be the neighbor of a pendent vertex of U, thus it obtains

$$SO(U) \geq (D-3)\sqrt{8} + \sqrt{5} + \sqrt{17} + \sqrt{20}. \tag{7}$$

Note that in this case, we have $D \geq 4$. Thus the relation (6) is smaller than (7) and we deduce that $SO(U) \geq (D-4)\sqrt{8} + 2\sqrt{5} + 2\sqrt{13}$. Also the graph G contains the cycle C_l which has a vertex of degree 3 or 4. Therefore, we have the following inequalities $SO(C_l) \geq (l-2)\sqrt{8} + 2\sqrt{13}$ or $SO(C_l) \geq (l-2)\sqrt{8} + 2\sqrt{20} > (l-2)\sqrt{8} + 2\sqrt{13}$. As a result, since $n = l + D$, we have

$$\begin{aligned} SO(G) &\geq SO(C_l) + SO(U) \geq (D+l-6)\sqrt{8} + 4\sqrt{13} + 2\sqrt{5} \\ &= (n-6)\sqrt{8} + 4\sqrt{13} + 2\sqrt{5} \geq SO(U_1). \end{aligned}$$

Subcase 2-3: When $P \cap P^{'} \neq \emptyset$ and there exists a diametral path U containing exactly one pendent vertex of the graph G.

Because one pendent vertex of G is not in U, by Lemma 1, there is a unicyclic graph $G^{'} \subset G$ containing exactly one pendent vertex of U such that $D(G) = D(G^{'})$ and $SO(G) > SO(G^{'})$. According to the Case 1, it implies that $SO(G^{'}) \geq SO(U_1)$.

Case3: The graph G has at least three pendent vertices.

Suppose that U be a diametral path of G. Obviously, this path contains at most two pendent vertices of G. Since G has $m \geq 3$ pendent vertices, thus at least $m-2$ pendent vertices are not in U. By Lemma 1, there is a unicyclic graph $G^{'} \subset G$ containing only the pendent vertices of U such that $D(G) = D(G^{'})$ and $SO(G) > SO(G^{'})$. With the same argument of the Case1, we obtain again that $SO(G^{'}) \geq SO(U_1)$. ■

Theorem 2. *Let G be a unicyclic graph with the diameter $D \geq 3$ and $n \geq 2D$. Then, $SO(G) \geq SO(U_2) = (n-3)\sqrt{8} + 2\sqrt{13} + \sqrt{10}$, where U_2 is the graph obtained from connected one pendent vertex to one vertex of C_{2D-1}.*

Proof. If G has exactly one pendent vertex, then $n = 2D$, thus $G \cong U_2$ and the claim is proven. Consider G has exactly two pendent vertices, so $n = 2D$ or $n = 2D+1$. If $n = 2D$, then there is a diametral path U such that this path contains only one pendent vertex of G. By Lemma 1, there is a unicyclic graph $G^{'} \subset G$ containing only the pendent vertex of U such that $D(G) = D(G^{'})$ and $SO(G) > SO(G^{'})$. Therefore we have

$$SO(G) > SO(G^{'}) \geq SO(U_2) = (n-3)\sqrt{8} + 2\sqrt{13} + \sqrt{10}.$$

If $n = 2D+1$, then G is the graph obtained from connected two pendent vertices to C_{2D-1}, hence if both pendent vertices are connected to one vertex of G, then

$$\begin{aligned} SO(G) &= (2D-3)\sqrt{8} + 2\sqrt{20} + 2\sqrt{17} = (n-4)\sqrt{8} + 2\sqrt{20} + 2\sqrt{17} \\ &\geq (n-3)\sqrt{8} + 2\sqrt{13} + \sqrt{10} = SO(U_2), \end{aligned}$$

and if pendent vertices are connected to two vertices of G, we deduce the following $SO(G) = (2D-4)\sqrt{8} + 2\sqrt{13} + 2\sqrt{10} + \sqrt{18}$ or $SO(G) = (2D-5)\sqrt{8} + 4\sqrt{13} + 2\sqrt{10}$.

Therefore,

$$\begin{aligned} SO(G) &\geq (2D-4)\sqrt{8} + 2\sqrt{13} + 2\sqrt{10} + \sqrt{18} \\ &= (n-5)\sqrt{8} + 2\sqrt{13} + 2\sqrt{10} + \sqrt{18} \\ &\geq (n-3)\sqrt{8} + 2\sqrt{13} + \sqrt{10} = SO(U_2). \end{aligned}$$

Otherwise, G has at least three pendent vertices and at most two pendent vertices are in the diametral path U. By Lemma 1, there exists a unicyclic graph $G^{'} \subset G$ containing only the pendent vertices of U such that $D(G) = D(G^{'})$ and $SO(G) > SO(G^{'})$. It obtains again that $SO(G) > SO(G^{'}) \geq SO(U_2)$. ■

Theorem 3. *Let G be a unicyclic graph with the diameter $D = 2$, then $SO(G) \geq 2D\sqrt{8}$.*

Proof. The unicyclic graphs G with the diameter $D = 2$, are either the cycle C_4 with the Sombor index $SO(G) = 4\sqrt{8}$, or the cycle C_5 with the Sombor index $SO(G) = 5\sqrt{8}$, and or a graph obtained from the cycle C_3 by connecting at least one pendent vertex to one vertex of C_3.

Let $V(C_3) = \{x_1, x_2, x_3\}$, and $y_1, y_2, \ldots, y_k$ are pendent vertices connected to x_1, then $x_2x_1y_1$ is a diametral path in G. By Lemma 1, there is a unicyclic graph $G^{'} \subset G$ containing only the pendent vertex y_1 such that $D(G) = D(G^{'})$ and $SO(G) > SO(G^{'})$. It holds $SO(G^{'}) = \sqrt{8}+2\sqrt{13}+\sqrt{5}$. Hence we prove that $SO(G) \geq 4\sqrt{8}$. ■

In [5], Gutman defined the reduced Sombor index of a graph G, replacing d_v by $d_v - 1$ for all $v \in V(G)$. Infact, the reduced Sombor index is the distances of isolated edegs with d-coordinate $(1, 1)$ and d-points of the graph G which given as $SO_{red}(G) = \sum_{uv \in E(G)} \sqrt{(d_u - 1)^2 + (d_v - 1)^2}$.

We have the similar result for the reduced Sombor index.

Theorem 4. *Let G be a unicyclic graph with n vertices and the diameter D such that $D \geq 3$ and $n \geq D + 2$. Then,*

$$SO_{red}(G) \geq SO_{red}(U_1) = (n-4)\sqrt{2} + 3\sqrt{5} + 1.$$

Moreover, if $D = 2$, then $SO_{red}(G) \geq 2D\sqrt{2}$. Furthermore, if $D \geq 3$ and $n \geq 2D$, we have $SO_{red}(G) \geq SO_{red}(U_2) = (n-3)\sqrt{2} + 2\sqrt{5} + 2$.

Proof. The proof is done with the same argument of the perivous theorems. ■

3 An application

One of the applications of topological indices is devoted to the study of some properties of chemical structures such as physical properties, chemical reactivity, or biological activity. Some samples of chemical unicyclic graphs are corresponding graphs of cyclic hydrocarbons such as the graph of 1-etyle-3-metylecyclopentane with the Sombor index $SO(G) = 5\sqrt{13} + \sqrt{10} + \sqrt{5} + \sqrt{8}$, the graph of methylcyclopentane with the Sombor index $SO(G) = 3\sqrt{8} + 2\sqrt{13} + \sqrt{10}$, the graph of Benzene with the Sombor index $SO(G) = 6\sqrt{8}$ and so on.

In this paper, we present minimum bounds on Sombor index of the unicyclic graphs with fixed diameter. These results could provide further information to show the advantages and limitations of topological type indices and related descriptors in Quantitative Structure-Activity Relationship (QSAR) or Quantitative Structure-Property Relationship (QSPR) studies for chemical (unicyclic) graphs and molecular structures.

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