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The Sombor Index of Unicyclic Graphs with given Diameter

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Abstract. The Somber index is a new vertex-degree-based topological index that introduced by Gutman on the chemical graphs. In this paper, we present the Sombor index of unicyclic graphs with given diameter.

Keywords: Sombor index, unicyclic graph, diameter

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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 $D(G) = \{max\ d(u, v) : u, v \in V(G)\}$. 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.

Gutman in [1] 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.

Li et al. [2] 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.

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Unicyclic graphs as one of the great classes can exhibit various chemical structures as well. Réti et al. [4] 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 [3] 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. Song and Pan in [5] obtained sharp lower bounds of Randić index of unicyclic graphs of a fixed order and diameter. Zhong [6] 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 Theorem 1.3. 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 1.1. *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

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

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

Lemma 1.2. *[4] Let G be a connected unicyclic graph with $n \geq 4$ vertices, then $SO(G) \geq SO(C_n) = n\sqrt{8}$.*

By Lemma 1.2, in this paper we will consider the unicyclic graphs with at least one pendent vertex.

Theorem 1.3. *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,

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

Let $m \geq 2$ and $l \geq 4$, then,

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

on the other hand, we have,

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

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

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 $SO(G) = SO(C_l) + SO(P) + SO(P^{'})$. Let $l \geq 4$ and $m_1, m_2 \geq 2$. Thus $SO(P) = (m_1-2)\sqrt{8} + \sqrt{13} + \sqrt{5}$, 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. 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. 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

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

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 1.1, 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 1.1, 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 1.4. *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 1.1, 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 $SO(G) \geq 4\sqrt{8}$. □

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