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# On the revised Szeged index

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ABSTRACT

We give bounds for the revised Szeged index, and determine the $n$-vertex unicyclic graphs with the smallest, the second-smallest and the third-smallest revised Szeged indices for $n \geq 5$, and the $n$-vertex unicyclic graphs with the $k$th-largest revised Szeged indices for all $k$ up to 3 for $n = 5$, to 5 for $n = 6$, to 6 for $n = 7$, to 7 for $n = 8$, and to $\lfloor \frac{n}{2} \rfloor + 4$ for $n \geq 9$. We also determine the $n$-vertex unicyclic graphs of cycle length $r$, $3 \leq r \leq n$, with the smallest and the largest revised Szeged indices.



## 1. Introduction

Topological indices are graph invariants used in theoretical chemistry to encode molecules for the design of chemical compounds with given physicochemical properties or given pharmacological and biological activities [25]. In this paper, we consider a topological index named the revised Szeged index, which is closely related to two other topological indices, the Wiener index and the Szeged index.

Let $G$ be a simple connected graph with vertex set $V(G)$ and edge set $E(G)$. Let $d_G(u, v)$ be the distance between vertices $u$ and $v$ in $G$. The Wiener index of $G$ is defined as [7]

$$W(G) = \sum_{\{u,v\} \subseteq V(G)} d_G(u, v).$$

It has been thoroughly studied; see, e.g., [5,6,1]. Besides of interest for the use in chemistry, it was also independently studied as of relevance for social science, architecture, and graph theory [22]. If $e$ is an edge of $G$ connecting vertices $u$ and $v$, then we write $e = uv$ or $e = vu$. For $e = uv \in E(G)$, let $n_1(e|G)$ and $n_2(e|G)$ be respectively the number of vertices of $G$ lying closer to vertex $u$ than to vertex $v$ and the number of vertices of $G$ lying closer to vertex $v$ than to vertex $u$. If $G$ is a tree, then it is known that $W(G) = \sum_{e \in E(G)} n_1(e|G) n_2(e|G)$; see [26]. Gutman [3] introduced, as a generalization of this relation, a graph invariant named the Szeged index. The Szeged index of a connected graph $G$ is defined as [3]

$$Sz(G) = \sum_{e \in E(G)} n_1(e|G) n_2(e|G).$$

The Szeged index has received much attention for both its mathematical and computational properties; see, e.g., [11,4,17, 2,27,24], and its various applications in modeling physicochemical properties as well as physiological activities of organic compounds acting as drugs or possessing pharmacological activity; see [14]. Recent results on the Szeged index may be

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found in [15,29,18], and, in particular, ordering of unicyclic graphs by their Szeged indices was studied in [29]. Related work may be found in [16]. The Szeged index is a vertex-multiplicative type of topological index that takes into account the way vertices of a graph are distributed. Recall that a similar topological index, the PI index, takes into account the distribution of edges of additive type [10,13], which has also been studied extensively; see, e.g., [9,12,19].

Considering contributions from vertices not considered in the definition of $Sz$, Randić [23] conceived a modified version of the Szeged index, which is named the revised Szeged index in [20,21], by dividing equally the count vertices at the same distance from both end vertices of an edge. The revised Szeged index of the graph $G$ is defined as [20,21,23]

$$Sz^*(G) = \sum_{e\in E(G)} \left(n_1(e|G) + \frac{n_0(e|G)}{2}\right)\left(n_2(e|G) + \frac{n_0(e|G)}{2}\right),$$

where $n_0(e|G)$ is the number of vertices with equal distances from both end vertices of the edge $e$. Some properties and applications of this graph invariant have been reported in [20,21,23].

In this paper, we establish further properties for the revised Szeged index. We give bounds for the revised Szeged index, and determine the $n$-vertex unicyclic graphs with the smallest, the second-smallest and the third-smallest revised Szeged indices for $n \geq 5$, and the $n$-vertex unicyclic graphs with the $k$th-largest revised Szeged indices for all $k$ up to 3 for $n = 5$, to 5 for $n = 6$, to 6 for $n = 7$, to 7 for $n = 8$, and to $\lfloor \frac{n}{2} \rfloor + 4$ for $n \geq 9$. We also determine the $n$-vertex unicyclic graphs of cycle length $r$, $3 \leq r \leq n$, with the smallest and the largest revised Szeged indices.

## 2. Preliminaries

Let $S_n$ and $P_n$ be respectively the $n$-vertex star and the $n$-vertex path. For a connected graph $G$ with $u \in V(G)$, let $D(u|G) = \sum_{v\in V(G)} d_G(u, v)$. For graph $G$ and $H$, $G = H$ means that $G$ and $H$ are isomorphic.

**Lemma 2.1** *([1]). Let $T$ be an $n$-vertex tree different from $S_n$ and $P_n$. Then $(n-1)^2 = W(S_n) < W(T) < W(P_n) = \frac{1}{6}(n^3 - n)$.*

We also need the following three lemmas, which are easy to verify; see also [28].

**Lemma 2.2.** *Let $T$ be an $n$-vertex tree with $u \in V(T)$, where $u$ is not the center if $T = S_n$ and $u$ is not a terminal vertex if $T = P_n$. Let $x$ and $y$ be the center of the star $S_n$ and a terminal vertex of the path $P_n$, respectively. Then $n - 1 = D(x|S_n) < D(u|T) < D(y|P_n) = \frac{1}{2}n(n-1)$.*

For $n \geq 5$, let $S_n'$ be the tree formed by attaching a pendant vertex to a pendant vertex of the star $S_{n-1}$, and for $n \geq 6$, $S_n''$ be the tree formed by attaching two pendant vertices to a pendant vertex of the star $S_{n-2}$.

**Lemma 2.3.** *Among the $n$-vertex trees, $S_n'$ for $n \geq 5$ and $S_n''$ for $n \geq 6$ are the unique trees with respectively the second-smallest and the third-smallest Wiener indices, which are equal to $n^2 - n - 2$ and $n^2 - 7$, respectively.*

**Lemma 2.4.** *Let $T$ be an $n$-vertex tree with $n \geq 6$, $u \in V(T)$, $T \neq S_n$, where $u$ is not the vertex of maximal degree if $T = S_n'$. Let $x$ and $y$ be the vertices of maximal degree in $S_n'$ and $S_n''$, respectively. Then $D(x|S_n') = n < D(y|S_n'') = n + 1 \leq D(u|T)$.*

Note that if $G$ is a bipartite graph, then $n_0(e|G) = 0$ for any edge $e$ of $G$ and thus $Sz^*(G) = Sz(G)$.

Let $\mathbb{U}_{n,r}$ be the set of $n$-vertex unicyclic graphs with cycle length $r$, where $3 \leq r \leq n$, and $\mathcal{U}_n$ be the set of $n$-vertex unicyclic graphs, where $n \geq 3$.

## 3. Revised Szeged indices of connected graphs

In this section, we give best possible lower and upper bounds for the revised Szeged index, and a formula for the revised Szeged index of unicyclic graphs.

Let $K_n$ be the $n$-vertex complete graph.

**Theorem 3.1.** *Let $G$ be a connected graph with $n$ vertices. Then*

$$(n-1)^2 \leq Sz^*(G) \leq \frac{n^3(n-1)}{8}$$

*with left equality if and only if $G = S_n$ and with right equality if and only if $G = K_n$.*

**Proof.** For $e \in E(G)$,

$$\left(n_1(e|G) + \frac{n_0(e|G)}{2}\right)\left(n_2(e|G) + \frac{n_0(e|G)}{2}\right) = \frac{n_1(e|G) + n - n_2(e|G)}{2} \cdot \frac{n_2(e|G) + n - n_1(e|G)}{2}$$
$$= \frac{n^2 - (n_1(e|G) - n_2(e|G))^2}{4}.$$