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Note

A Novel Version of the Edge-Szeged Index

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Abstract. A novel version of the edge-Szeged index is proposed in parallel to the revised (vertex) Szeged index, and some properties, especially lower and upper bounds are established for this molecular descriptor. (doi: 10.5562/cca1889)

Keywords: Szeged index, edge-Szeged index, revised edge-Szeged index, distance

INTRODUCTION

The Szeged index, denoted by *Sz*, has been introduced by Gutman[1] in 1994 whilst he was visiting the Attila József University in Szeged, attractive historical city in south-east Hungary, hence the name of this molecular descriptor. Since the Szeged index has immediately been recognized as interesting and useful molecular descriptor, many contributions appeared to report its mathematical properties (*e.g.*, References 2–9) and various applications to modeling the physicochemical properties and physiological activites of organic compounds. Khadikar *et al.*[10] succinctly summarized the applications of the Szeged index in the quantitative structure-property-activity-toxicity modeling. In that paper the authors also stated that the total number of publications on the Szeged index and its variants up to the time of preparation of the paper is about 120 and among them more than 60 are reporting various applications. All these papers are listed in their review.[10] Since the article by Khadikar *et al.*[10] appeared in 2005, many more contributions appeared, *e.g.*, References 11–15.

The study of the Szeged index and its variants, such as the hyper-Szeged index, PI index, Harary-Szeged index, edge-Szeged index, etc., in the structure-property-activity modeling was summarized besides in Reference 10 also in two comprehensive handbooks on molecular descriptors.[16,17] All these warrant further work on the Szeged index and its variants. In this report, we present a novel version of the edge-Szeged index.

PRELIMINARIES

Let G be a connected graph with vertex set $V(G)$ and edge set $E(G)$. For $u,v \in V(G)$, $d(u,v \mid G)$ denotes the distance between u and v in G.[18]

For $uv \in E(G)$, let $n_G(u,v)$ be the number of vertices closer to vertex u than vertex v and $n_G(v,u)$ the number of vertices closer to vertex v than vertex u, *i.e.*,

$$n_G(u,v) = |\{w \in V(G) : d(w,u \mid G) < d(w,v \mid G)\}|,$$
$$n_G(v,u) = |\{w \in V(G) : d(w,v \mid G) < d(w,u \mid G)\}|.$$

The Szeged index of a (molecular) graph G, $Sz(G)$, is defined as[1]

$$Sz(G) = \sum_{uv \in E(G)} n_G(u,v) n_G(v,u).$$

If G is a tree, then $Sz(G) = W(G)$, the Wiener index of G.[19]

Let $n_G(uv)$ be the number of vertices equidistant from both ends of $uv \in E(G)$, *i.e.*, $n_G(uv) = |\{w \in V(G) : d(w,u \mid G) = d(w,v \mid G)\}|$. The revised Szeged index of G is defined as[20]

$$Sz^*(G) = \sum_{uv \in E(G)} \left(n_G(u,v) + \frac{n_G(uv)}{2} \right) \left(n_G(v,u) + \frac{n_G(uv)}{2} \right).$$

Several properties for this index have been established, *e.g.*, References 20–23.

For $e = uv \in E(G)$, $w \in V(G)$, the distance between e and w in G is defined as $d(e,w \mid G) =$

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$\min\{d(u,w\,|\,G), d(v,w\,|\,G)\}$. Let $m_G(u,v)$ be the number of edges closer to vertex u than vertex v and $m_G(v,u)$ the number of edges closer to vertex v than vertex u, *i.e.*,

$$m_G(u,v) = |\,\{e \in E(G) : d(e,u\,|\,G) < d(e,v\,|\,G)\}\,|,$$

$$m_G(v,u) = |\,\{e \in E(G) : d(e,v\,|\,G) < d(e,u\,|\,G)\}\,|.$$

The edge-Szeged index of G is defined as[24]

$$Sz_e(G) = \sum_{uv \in E(G)} m_G(u,v) m_G(v,u).$$

For more work on this index, see References 24–28.

Let $m_G(uv)$ be the number of edges equidistant from both ends of $e = uv \in E(G)$, *i.e.*, $m_G(uv) = |\,\{e \in E(G) : d(e,u\,|\,G) = d(e,v\,|\,G)\}\,|$. Motivated by the reports on the revision of the Szeged index,[20,22] below we propose the revised edge-Szeged index of G, defined as

$$Sz_e^*(G) = \sum_{uv \in E(G)} \left(m_G(u,v) + \frac{m_G(uv)}{2} \right) \left(m_G(v,u) + \frac{m_G(uv)}{2} \right).$$

REVISED EDGE-SZEGED INDEX OF CONNECTED GRAPHS

Let S_n and P_n be respectively the star and the path on n vertices, and K_n the complete graph on n vertices. Note also the molecular graphs are necessarily connected graphs.[18]

Proposition 1. Let G be a connected graph with m edges. Then

$$\frac{m(2m-1)}{4} \le Sz_e^*(G) \le \frac{m^3}{4}$$

with left equality if and only if $\{m_G(u,v), m_G(v,u)\} = \{m-1, 0\}$ for any $uv \in E(G)$ and with right equality if and only if $m_G(u,v) = m_G(v,u)$ for any $uv \in E(G)$.

From Proposition 1, we immediately have

Corollary 1. Let G be a connected graph with n vertices. Then

$$\frac{(n-1)(2n-3)}{4} \le Sz_e^*(G) \le \frac{n^3(n-1)^3}{32}$$

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

REVISED EDGE-SZEGED INDEX OF TREES

Proposition 2. Let T be an n-vertex tree. Then

$$\begin{aligned} Sz_e^*(T) &= Sz_e(T) + \frac{1}{4}(n-1)(2n-3) \\ &= W(T) - \frac{1}{4}(n-1)(2n-1). \end{aligned}$$

Thus the study of the revised edge-Szeged index, like the edge-Szeged index and the Szeged index, for trees is equivalent to the study of the Wiener index. It is interesting to see what happens for graphs with cycles. The startpoint is naturally unicyclic graphs.

REVISED EDGE-SZEGED INDEX OF UNICYCLIC GRAPHS

Proposition 3. Let G be a unicyclic graph with n vertices. Then

$$Sz_e^*(G) \le \frac{n^3}{4}$$

with equality if and only if G is the cycle C_n.

Let $C_r(T_1, T_2, \ldots, T_r)$ be the unicyclic graph with cycle $C_r = v_1 v_2 \ldots v_r v_1$ such that the deletion of all edges on C_r results in r vertex-disjoint trees $T_1, T_2, \ldots, T_r$ with $v_i \in V(T_i)$. Let $S_n(t_1, t_2, \ldots, t_r)$ be the n-vertex unicyclic graph $C_r(T_1, T_2, \ldots, T_r)$, where T_i is the star on $t_i + 1$ vertices with center v_i for $i = 1, 2, \ldots, r$ and $\sum_{i=1}^{r} t_i = n - r$. Let $S_{n,3} = S_n(n-3, 0, 0)$ and $S_{n,4} = S_n(n-4, 0, 0, 0)$. Let $|\,G\,| = |\,V(G)\,|$ for a graph G.

To give a lower bound for the revised edge-Szeged index for unicyclic graphs, we need a lemma.

Lemma 1. For $n \ge 5$, let G be an n-vertex unicyclic graph with cycle length 3. Then

$$Sz_e^*(G) \ge \frac{3}{4}n^2 + \frac{5}{4}n - \frac{15}{4}$$

with equality if and only if $G = S_{n,3}$.

Proposition 4. For $n \ge 5$, let G be an n-vertex unicyclic graph. Then

$$Sz_e^*(G) \ge \begin{cases} \frac{1}{2}n^2 + \frac{23}{4}n - 15 & \text{for } n \ge 15 \\ \frac{3}{4}n^2 + \frac{5}{4}n - \frac{15}{4} & \text{for } n \le 15 \end{cases}$$

with equality if and only if $G = S_{n,3}$ for $n \le 14$, $G = S_{n,3}$ or $S_{n,4}$ for $n = 15$, and $G = S_{n,4}$ for $n \ge 16$.

CONCLUSIONS

Original version of the Szeged index and its variants found considerable application in structure-property-activity modeling.[10,16,17] Here we propose a novel version of the edge-Szeged index and its properties are discussed for several classes of (molecular) graphs.

Supplementary Materials. – Supporting informations to the paper are enclosed to the electronic version of the article. These data can be found on the website of *Croatica Chemica Acta* (http://public.carnet.hr/ccacaa).

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