

The Edge Version of the Szeged Index

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The Szeged index is a molecular structure descriptor equal to the sum of products $n_u(e|G) \cdot n_v(e|G)$ over all edges $e = (uv)$ of the molecular graph G , where $n_u(e|G)$ is the number of vertices whose distance to vertex u is smaller than the distance to vertex v , and where $n_v(e|G)$ is defined analogously. We now examine the edge version of the Szeged index: the sum of products $m_u(e|G) \cdot m_v(e|G)$ over all edges $e = (uv)$ of the molecular graph G , where $m_u(e|G)$ is the number of edges whose distance to vertex u is smaller than the distance to vertex v , and where $m_v(e|G)$ is defined analogously. The basic properties of this novel structure descriptor are established. Most of these are analogous to the properties of the ordinary Szeged index, but some remarkable differences are also recognized.

INTRODUCTION

In Harold Wiener's seminal paper¹ a method is proposed for computing the structure-descriptor W (that nowadays is known under the name *Wiener index*). Wiener's method can be expressed by means of the formula

$$W(G) = \sum_e n_u(e|G) \cdot n_v(e|G); \quad G \text{ acyclic.} \quad (1)$$

The meaning of the symbols used in Eq. (1) is explained in due detail a few lines below.

Formula (1) may be viewed as the first theorem in the theory of the Wiener index (and probably as the first theorem for any molecular structure descriptor). Although Wiener's paper¹ was much quoted, his result (1) remained unnoticed for many years and seems to be first time explicitly stated (and proved) in the book.²

Formula (1) is valid for acyclic (molecular) graphs. One obvious question is what would happen if one would

apply it to cyclic graphs. Research along these lines led to the concept of Szeged index.³

We now provide the necessary definitions.

Let G be a (molecular) graph^{2,4} possessing n vertices and m edges. If e is an edge of G , connecting the vertices u and v , then we write $e = (uv)$. If G is a connected graph and x and y are two of its vertices, then the distance $d(x,y) = d(x,y|G)$ between the vertices x and y is equal to the length of the shortest path that connects them in G . The Wiener index $W(G)$ of a connected graph G is equal to the sum of distances between all pairs of vertices of G .

Let $e = (u,v)$ be an edge of the graph G . The number of vertices of G whose distance to the vertex u is smaller than the distance to the vertex v is denoted by $n_u(e) = n_u(e|G)$. Analogously, $n_v(e) = n_v(e|G)$ is the number of vertices of G whose distance to the vertex v is smaller than the distance to the vertex u . Note that vertices equidistant to u and v are not counted.

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By this, the meaning of all symbols occurring in Eq. (1) has been clarified. In Eq. (1) the summation goes over all edges of the graph G .

As already mentioned, Eq. (1) is valid only for trees (= connected acyclic graphs). A proper generalization of this equation was to conceive a new quantity,³ denoted here by $Sz_v = Sz_v(G)$:

$$Sz_v(G) = \sum_e n_u(e|G) \cdot n_v(e|G); \quad G \text{ any graph} \quad (2)$$

so that, by definition, Eq. (2) holds for all graphs. The new molecular structure descriptor was eventually named⁵ the Szeged index (and denoted by Sz), but for reasons explained below we refer to it as the vertex-Szeged index. It could be shown^{3,5-8} that Sz_v possesses mathematically non-trivial and chemically interesting properties; details of the theory and applications of the vertex-Szeged index can be found in the review⁹ and book.¹⁰

Motivated by the success of the Szeged index, Khadikar proposed a seemingly similar molecular structure descriptor,¹¹ that in what follows we call the edge-PI index. In analogy with Eq. (2), the edge-PI index is defined as

$$PI_e = PI_e(G) = \sum_e [m_u(e|G) + m_v(e|G)] \quad (3)$$

where the quantities $m_u(e|G)$ and $m_v(e|G)$ are the edge-variants of the numbers $n_u(e|G)$ and $n_v(e|G)$. More precisely: if $e' = (st)$ is an edge and x a vertex of the (connected) graph G , then the distance between e' and x is equal to $\min\{d(s,x), d(t,x)\}$. Then for $e = (uv)$ being an edge of the graph G , $m_u(e) = m_u(e|G)$ is the number of edges of G whose distance to the vertex u is smaller than the distance to the vertex v . Analogously, $m_v(e) = m_v(e|G)$ is the number of edges of G whose distance to the vertex v is smaller than the distance to the vertex u . Note that edges equidistant to u and v are not counted. For the theory and applications of the edge-PI index see the papers¹²⁻¹⁴ and the references quoted therein.

Quite recently the vertex-version of the PI index was also considered,¹⁵ defined as

$$PI_v = PI_v(G) = \sum_e [n_u(e|G) + n_v(e|G)]. \quad (4)$$

There is an evident symmetry between Eqs. (3) and (4), namely Eq. (3) may be viewed as the edge-version, whereas Eq. (4) as the vertex-version of the PI index. Following an analogous reasoning, we may understand Eq. (2) as the vertex-version of the Szeged index, and then its edge-version is readily conceived:

$$Sz_e(G) = \sum_e m_u(e|G) + m_v(e|G). \quad (5)$$

The purpose of this work is to examine this edge-Szeged index and establish its main properties.

THE EDGE-SZEGED INDEX OF TREES

Recalling the well known relation³

$$Sz_v(T) = W(T) \quad (6)$$

that holds for any tree T , and the fact that a tree with n vertices has $n-1$ edges, it is easy to find the expression for the edge-Szeged index of a tree, analogous to Eq. (6). Indeed, because for any edge $e = (uv)$, $m_u(e|T) = n_u(e|T) - 1$ and $m_v(e|T) = n_v(e|T) - 1$, we have

$$Sz_e(T) = \sum_e [n_u(e|T) - 1][n_v(e|T) - 1] = Sz_v(T) - \sum_e [n_u(e|T) + n_v(e|T) - 1].$$

In the case of trees (and, in general, of any n -vertex bipartite graph),³ $n_u(e|T) + n_v(e|T) = n$, and therefore

$$Sz_e(T) = Sz_v(T) - n(n-1) + (n-1)$$

which, in view of Eq. (6), finally yields

$$Sz_e(T) = W(T) - (n-1)^2. \quad (7)$$

Formula (7) can be written also in the form

$$Sz_e(T) = W(T) - W(S_n) \quad (8)$$

where S_n denotes the n -vertex star^{2,4} (whose Wiener index is known¹⁶ to be equal to $(n-1)^2$). From (8) it immediately follows that the edge-Szeged index of the star is equal to zero.

In fact, if G is any simple connected graph (with at least two vertices), then $Sz_e(G) = 0$ if and only if G is a star. To see this, observe that the product $n_u(e) \cdot n_v(e)$, occurring on the right-hand side of Eq. (5), is either positive or equal to zero. It is equal to zero only if either $n_u(e) = 0$ or $n_v(e) = 0$, which only happens if e is a pendent edge (an edge, one of whose vertices has degree 1). Therefore, $Sz_e(G) = 0$ if and only if all edges of the graph G are pendent, which in the case of connected graphs implies that all vertices of G , except one, are of degree 1. Evidently, the star is the only graph satisfying such a requirement.

By the above analysis we established a noteworthy property of the edge-Szeged index: it represents certain structural features of the internal edges (*i. e.*, of the non-pendent edges) of a (molecular) graph, whereas pendent edges make no contribution to Sz_e . This seems to be a significant difference in the structure-dependency of the vertex- and edge-versions of the Szeged index.

SOME FURTHER EXAMPLES

Directly from the definition (5), we calculate expressions for edge-Szeged index of the n -vertex complete graph (K_n), the complete bipartite graph ($K_{a,b}$) on $a + b$ verti-

ces, and the n -vertex cycle (C_n). For comparative reasons we report also the respective expressions⁶ for the vertex-Szeged index.

$$Sz_e(K_n) = \frac{1}{2}n(n-1)^3 \quad ; \quad Sz_v(K_n) = \frac{1}{2}n(n-1) \quad (9)$$

$$Sz_e(K_{a,b}) = ab(a-1)(b-1) \quad ; \quad Sz_v(K_{a,b}) = (ab)^2.$$

In particular, if $n = a + b$ is even, then

$$\begin{aligned} Sz_e(K_{n/2,n/2}) &= \frac{1}{16}n^2(n-2)^2 \quad ; \\ Sz_v(K_{n/2,n/2}) &= \frac{1}{16}n^4 \end{aligned} \quad (10)$$

whereas if $n = a + b$ is odd, then

$$\begin{aligned} Sz_e(K_{(n-1)/2,(n+1)/2}) &= \frac{1}{16}(n-1)^2(n+1)(n-3) \quad ; \\ Sz_v(K_{(n-1)/2,(n+1)/2}) &= \frac{1}{16}(n^2-1)^2. \end{aligned} \quad (11)$$

If n is even, then

$$Sz_e(C_n) = \left(\frac{n-2}{2}\right)^2 n \quad ; \quad Sz_v(C_n) = \left(\frac{n}{2}\right)^2 n.$$

If n is odd, then

$$Sz_e(C_n) = \left(\frac{n-1}{2}\right)^2 n \quad ; \quad Sz_v(C_n) = \left(\frac{n-1}{2}\right)^2 n.$$

It has been shown⁷ that among n -vertex graphs, the complete bipartite graph $K_{n/2,n/2}$ (if n is even) or $K_{(n-1)/2,(n+1)/2}$ (if n is odd) has the greatest vertex-Szeged index. By comparing the formulas (9), (10), and (11) we see that this cannot be the case with the edge-Szeged index, since $Sz_e(K_n)$ is greater than the edge-Szeged index of any n -vertex complete bipartite graph.

At this point we put forward the following:

Conjecture. The complete graph K_n has the greatest edge-Szeged index among all n -vertex graphs.

EDGE-SZEGED INDEX OF BENZENOID SYSTEMS

The vertex-Szeged index of benzenoid systems can be computed by considering its elementary (or orthogonal)¹⁴ cuts. An elementary cut is a line segment that starts at the center of a peripheral edge of a benzenoid system B , goes orthogonal to it and ends at the first next peripheral edge of B . Details on elementary cuts can be found elsewhere.^{8,14,17-20} In what follows we denote an elementary cut by C and the number of edges that it intersects by $|C|$.

The formula for the vertex-Szeged index of a benzenoid system B reads:⁸

$$Sz_v(B) = \sum_C |C| n_1(C) \cdot n_2(C) \quad (12)$$

where $n_1(C)$ and $n_2(C)$ are numbers of vertices lying on the two sides of the elementary cut C , and where the summation goes over all elementary cuts of B . Note that⁸ $n_1(C) + n_2(C) = n$ for all elementary cuts.

By means of a reasoning that is fully analogous to what was used⁸ for the derivation of formula (12), we obtain

$$Sz_e(B) = \sum_C |C| m_1(C) \cdot m_2(C) \quad (13)$$

where now $m_1(C)$ and $m_2(C)$ count the edges on the two sides of C . A minor difference between Eqs. (12) and (13) is that the sum $m_1(C) + m_2(C)$ is not independent of the cut C . Indeed, $m_1(C) + m_2(C) + |C| = m$, because the edges of B either lie on one or on the other side of the elementary cut C , or are intersected by C .

Eq. (13) makes the calculation of the edge-Szeged index of benzenoid systems rather easy. Instead of illustrating this by some simple examples, we state the general expression for the relation between the edge- and vertex-Szeged indices of a catacondensed benzenoid system possessing h hexagons:

$$\begin{aligned} Sz_e = \\ \frac{1}{16} \left[25Sz_v - (5h+1)(60h+21) - (40h+8) \sum_C |C|^2 + 4 \sum_C |C|^3 \right]. \end{aligned} \quad (14)$$

Formula (14) may serve as a convincing illustration of the fact that the vertex- and the edge-Szeged indices of polycyclic molecular graphs have quite different structure-dependence, and thus reflect different structural features of the underlying molecules. This observation may be a motivation for applying Sz_e (in addition to Sz_v)¹⁰ in molecular-structure-descriptor-based QSPR/QSAR studies.

As a final remark we mention that formula (13), as well as formula (12), is applicable not only to benzenoid systems, but also to phenylenes^{21,22} and other related polycyclic molecular graphs.

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SAŽETAK

Inačica Szegedskog indeksa zasnovana na bridovima grafa

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Szegedski indeks je molekularni strukturni deskriptor jednak zbroju produkata $n_u(e | G) \cdot n_v(e | G)$ preko svih bridova $e = (uv)$ molekularnog grafa G , gdje je $n_u(e | G)$ broj vrhova čije je rastojanje od vrha u manje nego rastojanje od vrha v , i gdje je $n_v(e | G)$ definiran analogno. U ovom radu istražujemo inačicu Szegedskog indeksa zasnovanu na bridovima grafa: zbroj produkata $m_u(e | G) \cdot m_v(e | G)$ preko svih bridova $e = (uv)$ molekularnog grafa G , gdje je $m_u(e | G)$ broj bridova čije je rastojanje od vrha u manje nego rastojanje od vrha v , i gdje je $m_v(e | G)$ definiran analogno. Ustanovljena su osnovna svojstva ovog novog strukturnog deskriptora. Mnoga od njih su analogna onima običnog Szegedskog indeksa, ali postoje i značajne razlike.