Szeged Index: Formulas For Fused Bicyclic Graphs

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The Szeged index \( Sz \) is a variant of the well known Wiener index \( W \). It has been shown that \( Sz(B_N) \) is a third order polynomial in terms of the sizes of three chains making up a fused bicyclic graph \( B_N \). Analytical formulas have been derived for \( Sz(B_N) \).

INTRODUCTION

The Szeged index \( Sz \) is a graph invariant which was introduced by Gutman.\(^1\) Its definition is based on the original definition of the well known Wiener index.\(^2\) According to this definition for an acyclic graph \( T \) (where \( T \) refers to a tree, in Wiener’s paper an acyclic hydrocarbon), \( W(T) \) is equal to the sum of «bond contributions»:

\[
W(T) = \sum_{(a,b)} n_a \times n_b
\]

where \( a \) and \( b \) are adjacent vertices of \( T \) and \( (a,b) \) denotes the edge connecting vertices \( a \) and \( b \), \( n_a \) and \( n_b \) denote the number of vertices in the respective disconnected graphs obtained by removing edge \( (a,b) \) from \( T \). Only carbons are considered, hydrogens are neglected. The definition is valid for trees only.

The original definition given by Wiener could be extended to any graph \( G \), including cycle-containing graphs, by using the fact (which was also found out by Wiener) that \( W(G) \) is equal to the sum of distances between all pairs of vertices.

\[
W(G) = \sum_{(i<j)} D_{i,j}
\]
Eq. (2) is Hosoya’s formula, where $D_{ij}$ denotes the length of the shortest path between vertices $i$ and $j$. The entries $D_{ii}$ are zero.

Since Eq. (2) may be used for cycle-containing structures, and because of its simplicity, Hosoya’s equation, Eq. (2), is used when $W$ has to be calculated. It has to be noted that, many years after Wiener’s paper had appeared, the «bond-contribution» picture (Eq. (1)) could be extended for cycle-containing structures, too. It was shown that $W$ can be computed as a sum of bond contributions (i.e. $W = \sum W_e$, where $W_e$ denotes the contribution of bond $e$ and the summation has to be performed for all bonds), and each bond-contribution term is equal to

$$W_e = \sum_{ij} \frac{K_e}{K_{ij}}$$

where $K_{ij}$ denotes the number of shortest paths between vertices $i$ and $j$ which contain $e$ and $K_{ij}$ is the total number of the shortest paths between $i$ and $j$.

Gutman proposed a different interpretation of the «bond-contribution» approach (Eq. (1)). In his approach Eq. (1) remains valid but the definitions of $n_a$ and $n_b$ are replaced by the following formulas:

$$n_a = |\{x|D_{x,a} < D_{x,b}\}|$$

and

$$n_b = |\{x|D_{x,b} < D_{x,a}\}|.$$

According to Eq. (4), $n_a$ is the number of vertices (including vertex $a$ itself) nearer to vertex $a$ than to $b$, and a similar definition holds for $n_b$ (Eq. (5)). Note that vertices $x$ for which $D_{x,a} = D_{x,b}$ will not be considered.

The third variant of $W$, being equivalent to $W$ in trees but different from it in cycle-containing graphs, is the detour index $w$. $w$ may be obtained by using an analogue of Eq. (2) in which the distances $D_{ij}$ are replaced by entries $\Delta_{ij}$, i.e. by the lengths of the longest paths between vertices $i$ and $j$.

The fourth possibility of extending $W$ to cyclic structures might be accomplished by observing the fact that in trees the sum of the positive eigenvalues of the Laplacian matrix $L$ is equal to $W$. Therefore the new invariant, being the sum of positive eigenvalues of $L(G)$, would be equivalent to $W$ in trees, but would be different from it in cycle-containing graphs.

In 1994, Randić introduced the «hyper-Wiener index» $WW$ by modifying Wiener’s definition. Originally, $WW$ could only be obtained for acyclic graphs but it was later shown that $WW$ may be obtained for cycle-containing graphs $G$, too, by using the following formula.
\[ WW(G) = \frac{1}{2} \sum_{i \neq j} (D_{ij} + D_{ij}^2). \]  

Later on, the »hyper» variants of \( Sz \) and \( w \) were also introduced.\(^{13,14}\)

A further variant of \( W \) was proposed by Rouvray,\(^{15}\) but it was found later on that this index is equal to \( 2W \). An expanded version of \( W \) was introduced by Tratch \textit{et al.},\(^{16}\) in which for each pair of vertices \( i \) and \( j \), the distance \( D_{ij} \) is multiplied by the number of »superpaths« containing the corresponding shortest path between \( i \) and \( j \), and the products are added. In cycle-containing structures each product has to be multiplied by the number of shortest \( i-j \) paths. A special version of \( W \) is based on the »resistance distance« model and another one on asymmetric matrices that were obtained from the distance matrix.\(^{17}\) The mathematical aspects and numerous applications of \( W \) have been reviewed several times.\(^{19-22}\) A special review was devoted to the distance matrix.\(^{23}\)

Because of the importance of \( W \), other closely related graph invariants, like the Szeged (and the detour) index, are also interesting. In fact, many interesting mathematical properties of \( Sz \) have been discovered thus far.\(^{24-29}\) In particular, it has been demonstrated that \( Sz(G) = W(G) \) if and only if every block of \( G \) is a complete graph.\(^{29}\) The aim of the present paper is to show that \( Sz \) is a third order polynomial in terms of the sizes of chains making up a fused bicyclic graph. Formulas for \( N \) vertex fused bicyclic graphs \( B_N \) (Figure 1) have been derived. \( Sz \) is also in this respect related to \( W \), \( w \), \( WW \) and the hyper detour index, for which analytical formulas were obtained earlier and these are also polynomials.\(^{14,30-37}\)

![Figure 1. An example of a fused bicyclic graph with \( k = 8 \), \( m = 6 \) and \( n = 4 \).](image)

**DERIVATION OF THE POLYNOMIAL**

Expressions like »graph« and »structural formula«, »valence« and »degree« are synonyms. Therefore, corresponding expressions used in chemistry and in graph theory, like »chemical bond« and »edge«, »atom« and »vertex«
will be used interchangeably hereafter. A »graph invariant« is the number which depends on graph G but does not depend on the numbering of the vertices in G. Hydrogen suppressed graphs will be considered only.

First, it has to be shown that $Sz(B_N)$ is a polynomial. Consider an example of a fused bicyclic graph $B_N$ (Figure 1). There are three chains – subgraphs of $B_N$ – $k, m$ and $n$, which connect the branching vertices. $k, m$ and $n$ include the branching vertices. Examples: 1. The (hydrogen suppressed) graph of ethane is a single chain consisting of two vertices (endpoints), 2. The (hydrogen suppressed) graph of isobutane consists of three chains, each containing two vertices (the branching atom and the endpoint). Since branching vertices are considered several times in $B_N$, the total number of vertices $N$ is therefore equal to $k+m+n-4$. Note that throughout this paper letters $k, m$ and $n$ will be used to denote the respective chains and the number of vertices (which will be referred to as the «size» of the chain) in $k, m$ and $n$, respectively. Throughout this paper it will be assumed that $k \geq m \geq n$.

Figure 1 illustrates a special case but the procedure can easily be applied to any $B_N$. Bonds (12,1), (1,2), (2,3) and (3,4) will be considered only; a similar procedure could be used for the rest of the bonds of chain $k$ and for $m$ and $n$. Observe that $k+n-2$ denotes the size of a cycle. Two cases will be distinguished.

**Case 1:** $i+n-1 < (k+n-2)/2$, where the running index $i$ refers to the first figures in the parentheses. Then for bonds (12,1) and (1,2): $n_a = (k+n-2)/2+m-2 = 9$ and $n_b = (k+n-2)/2 = 5$, where $n_a$ refers to the first figure in the parentheses and $n_b$ to the second.

**Case 2:** $i+n-1 \geq (k+n-2)/2$. For bonds (2,3) and (3,4), the following expressions are valid: $n_a = (2k+m+n-4)/2-i-1$, and $n_b = (2k+m+n-4)/2-(k-i-1)$.

In general, in the first case the first vertex is nearer to the both branching vertices than the second, and in the second case the second vertex is nearer to one of the branching vertices than the first one.

The product $n_an_b$ is a second order polynomial in terms of $k, m, n$ and $i$. The sum of these products is a third order polynomial in terms of numbers $k, m$ and $n$ and the running index $i$ drops out. $Sz(B_N)$ is therefore a polynomial in terms of $k, m$ and $n$. Although the derivation was given for a special case, where $k, m$ and $n$ are even, the procedure can be performed for other cases as well. The following theorem ensures that $Sz(B_N)$ is always a third order polynomial.

**THEOREM.**

$$Sz(B_N) \leq N^2(N+1)/4$$ (7)

**Proof.** The proof uses a result by Dobrynin\(^{38}\) according to which for any graph $G$, and therefore also for $B_N$:
\[ Sz(B_N) = 0.25 \left( \sum_{(a,b)} (N-n_{ab})^2 - \sum_{(a,b)} (n_a-n_b)^2 \right) \] (8)

where \( n_{ab} \) is the number of vertices being equally far from \( a \) and \( b \). But:

\[ Sz(B_N) \leq 0.25 \sum_{(a,b)} (N-n_{ab})^2 \leq 0.25 \sum_{(a,b)} N^2 = 0.25N^2(N+1). \] (9)

Q.E.D.

Because of this result, \( Sz(B_N) \) cannot be a fourth order polynomial in terms of \( k, m \) and \( n \), unlike the Szeged index of a complete bipartite graph which is a fourth order polynomial\(^{38}\) in terms of \( N \).

Derivation of the formulas \( Sz(B_N) \) in terms of \( k, m \) and \( n \) was done by solving a system of 20 simultaneous linear equations with 20 unknowns \( (A, B...T) \).

\[ Sz(B_N) = Ak^3 + Bm^3 + Cn^3 + Dk^2m + Ek^2n + Fm^2n + \]
\[ + Gm^2k + Hn^2k + In^2m + Jkmn + Kk^2 + Lm^2 + Mn^2 + \]
\[ + Nkm + Okn + Pmn + Qk + Rm + Sn + T. \] (10)

The equations were solved for known values of \( Sz(B_N) \) and by using the values of \( k^3, m^3, n^3, k^2m, \text{etc.} \) and of course the result cannot depend on the special choice of \( k, m \) and \( n \) values. Quite often, however, the matrix composed of powers of \( k, m \) and \( n \) is singular, therefore we have listed those combinations of the values of \( k, m \) and \( n \), which did not yield a singular matrix (Table I). The values of \( Sz \) were obtained by using an algorithm similar to that proposed by Žerovnik.\(^{39}\)

Case I. \( k, m \) and \( n \) are even, or \( k, m \) and \( n \) are odd.

\[ Sz(B_N) = (k^3 + m^3 + 2k^2m + 4k^2n + 4m^2n + 2m^2k + 3n^2k + \]
\[ + 8n^2m + 2k^2mn - 14k^2 - 14n^2 - 8k^2 - 22km - 26kn - 26mn + \]
\[ + 36k + 36m + 46n - 48)/4. \] (11)

Case II. \( k \) and \( m \) are even and \( n \) is odd, or \( k \) and \( m \) are odd and \( n \) is even.

\[ Sz(B_N) = (k^3 + m^3 + 2k^2m + 4k^2n + 4m^2n + 2m^2k + 3n^2k + \]
\[ + 8n^2m + 2k^2mn - 14k^2 - 14n^2 - 8k^2 - 22km - 32kn - 32mn + \]
\[ + 65k + 65m + 60n - 102)/4. \] (12)

Case III. \( k \) is even and \( m \) and \( n \) are odd or \( k \) is odd, and \( m \) and \( n \) are even.
TABLE I

List of paths and the respective values of \( S_z \) used to derive formulas 11–14.

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\[ S_2(B_N) = (k^3 + m^3 + 2k^2m + 4k^2n + 4m^2n + 2m^2k + 3n^2k + \]
\[ + 3n^2m + 6kmn - 13k^2 - 12m^2 - 11n^2 - 18km - 32kn - 34mn + \]
\[ + 55k + 56m + 76n - 99)/4. \quad (13) \]

Case IV. \( k \) and \( n \) are even and \( m \) is odd or \( k \) and \( n \) are odd and \( m \) is even.

\[ S_2(B_N) = (k^3 + m^3 + 2k^2m + 4k^2n + 4m^2n + 2m^2k + 3n^2k + \]
\[ + 3n^2m + 6kmn - 12k^2 - 13m^2 - 11n^2 - 18km - 34kn - 32mn + \]
\[ + 56k + 55m + 76n - 99)/4. \quad (14) \]

**DISCUSSION**

All equations were derived by using one set of conditions imposed on \( k, m \) and \( n \) (e.g., even values of \( k, m \) and \( n \) were used to derive Eq. (11)), but they remain valid for the second set of conditions as well (in case I, for \( k, m \) and \( n \) are odd). Similarly, Eqs. (12)–(14) are also valid for cases fulfilling the respective second sets of conditions. Example: calculate \( S_2(k,m,n) \) for \( k = 9, m = 7 \) and \( n = 5 \). By using Eq. (11), we obtain

\[ S_2(9,7,5) = (9^3 + 7^3 + 2*9^2*7 + 4*9^2*5 + 4*7^2*5 + 2*7^2*9 + 3*5^2*9 + \]
\[ + 3*5^2*7 + 6*9*7*5 - 11*9^2 - 11*7^2 - 8*5^2 - 14*9*7 - 26*9*5 - \]
\[ - 26*7*5 + 36*9 + 36*7 + 46*5 - 48)/4 = (729 + 343 + 1134 + 1620 + \]
\[ + 980 + 882 + 675 + 525 + 1890 - 891 - 539 - 200 - 882 - 1170 - \]
\[ - 910 + 324 + 252 + 230 - 48)/4 = 4944/4 = 1236. \]

Observe that restrictions imposed in Case I and Case II are equivalent with the statements that the number of vertices is even or odd in both cycles, respectively. In Case III the number of vertices \((k+n-2)\) is odd in the larger cycle and even \((m+n-2)\) in the smaller cycle, and in Case IV. \( k+n-2 \) is even and \( m+n-2 \) is odd.

Eq. (11) remains valid if \( k = m = n = 1 \), and \( S_2(1,1,1) = 0 \). This graph corresponds to a «hypothetical methane» with a single vertex and three edges starting and ending at this vertex. Because \( S_2(1,1,1) = 0 \), the sum of the coefficients of Eq. 11 must be zero. In fact \( 1+1+2+4+4+2+3+3+6-11-11-8-14-26-26+36+36+46-48 = 0 \).

Comparison of the coefficients of Eqs. (11)–(14) shows that the coefficients of the third order terms are equal. In contrast, in equations obtained for \( W(B_N) \) and \( w(B_N) \), the coefficients of the second order terms are also equal.\(^{33,35}\) Note that \( n^3 \) does not appear in Eqs. (11)–(14).
A formula for $Sz(C_N)$, where $C_N$ denotes an $N$ vertex cycle, may be derived easily:

$$Sz(C_N) = N(N-1)^2/4 \quad (N \text{ is odd})$$  \hspace{1cm} (15)

and

$$Sz(C_N) = N^3/4 \quad (N \text{ is even}).$$  \hspace{1cm} (16)

Comparison of these formulas with Eqs. (11) and (13) reveals that $Sz(C_N)$ is not equal to $Sz(B_N)$ with $k = N$, and $m = n = 2$, whereas $W(C_N) = W(N,2,2)$, and also $w(C_N) = w(N,2,2).^{33,35}$

Eqs. (11)–(14) can easily be programmed. The result is an example of algebraic expressions derived by using a numerical method. Formulas of graph invariants may be applied to solve – at least within a given set of structures – the inverse »QSPR problem«, namely to find structures corresponding to a numerical value of graph invariant.\textsuperscript{40,41}

REFERENCES


**SAŽETAK**

**Szegedov indeks: formule za kondenzirane bicikličke grafove**

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Szegedov indeks (Sz) varijanta je poznatog Wienerova indeksa W. Pokazano je da je Sz(B_N) polinom trećeg reda u veličinama triju lanaca koji grade kondenzirani biciklički graf B_N. Izvedene su analitičke formule za Sz(B_N).