The zig-zag chain as an extremal value of VDB topological indices of polyomino chains

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Abstract

We give conditions on the numbers $\{\varphi_{ij}\}$ under which a vertex-degree-based topological index TI of the form

$$TI(G) = \sum_{1 \leq i \leq j \leq n-1} m_{ij}\varphi_{ij},$$

where G is a graph with n vertices and m_{ij} is the number of ij-edges, has the zigzag chain as an extreme value among all polyomino chains. As a consequence, we deduce that over the polyomino chains, the zigzag chain has the maximal value of the Randić index, the sum-connectivity index, the harmonic index and the geometric-arithmetic index, and the minimal value of the first Zagreb index, second Zagreb index and atom-bond-connectivity index.

1 Introduction

A vertex-degree-based topological index TI is defined from any set of real numbers $\{\varphi_{ij}\}$ as

$$TI(G) = \sum_{1 \leq i \leq j \leq n-1} m_{ij}\varphi_{ij}, \tag{1}$$

where G is a graph with n vertices, m_{ij} is the number of ij-edges, i.e. edges with end vertices of degree i and j. Many important topological indices are of this type, for instance, the first Zagreb index is obtained by setting $\varphi_{ij} = i + j$

[6], in the second Zagreb index $\varphi_{ij} = ij$ [6], in the Randić index $\varphi_{ij} = \frac{1}{\sqrt{ij}}$ [16], in the harmonic index $\varphi_{ij} = \frac{2}{i+j}$ [22], in the geometric-arithmetic index $\varphi_{ij} = \frac{2\sqrt{ij}}{i+j}$ [17], in the sum-connectivity index $\varphi_{ij} = \frac{1}{\sqrt{i+j}}$ [21], in the atom-bond-connectivity index $\varphi_{ij} = \sqrt{\frac{i+j-2}{ij}}$ [4] and in the augmented Zagreb index $\varphi_{ij} = \left(\frac{ij}{i+j-2}\right)^3$ [5]. For recent results on VDB topological indices we refer to ([2],[3],[7],[8],[13],[14]).

Topological indices over polyomino systems have appeared recently in the literature ([1],[9],[10],[11],[15], [18], [19], [20]). In this paper we continue the study of VDB topological indices over the class of polyomino systems initiated in [15]. Recall that a polyomino system is a finite 2-connected plane graph such that each interior face (also called cell) is surrounded by a regular square of length one. The inner dual graph of a polyomino P is defined as a plane graph in which the vertex set is the set of all cells of P and two vertices are adjacent if the corresponding two cells have an edge in common. A polyomino chain is a polyomino system whose inner dual graph is a path. A kink of a polyomino chain is any angularly connected square. A segment of a polyomino chain is a maximal linear chain including the kinks and/or terminal squares at its end. The number of squares in a segment its called the length of the segment. In particular, a zig-zag chain is a polyomino chain in which every segment has length 2 . We will denote by Z_n the zig-zag chain with n squares.

In [15] it was shown that under certain conditions on the numbers $\{\varphi_{ij}\}$, the value of a TI induced by $\{\varphi_{ij}\}$ is monotonely increasing (or decreasing) with respect to linearizing operations performed to an angularly connected square, implying that the linear chain is an extremal value for many of the well-known vertex-degree-based topological indices. In this paper we introduce new operations applied to a linear square of a polyomino chain, which guarantees a monotone increasing (or decreasing) TI-value. As a consequence, we show that the zig-zag chain is an extremal value of the VDB topological indices mentioned above, except for the augmented Zagreb index.

2 Variation of VDB topological indices under angularizing operations of polyomino chains

We compute in our following results the variation of a topological index of the form (1) under angularizing operations. If U is a polyomino chain and M is a subset of $E(U)$, then we denote by $E(U)\backslash M$ the set of edges in $E(U)$ that do not belong to M.

Lemma 2.1 *Let TI be a topological index induced by the numbers $\{\varphi_{ij}\}$. Consider the angularizing operation 1 shown in Figure 1, where X is a polyomino*

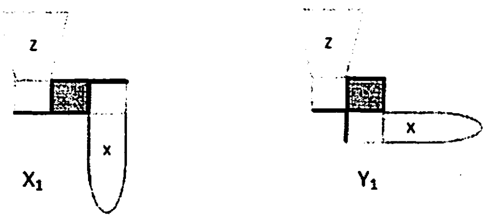

Figure 1: Angularizing operation 1.

chain and Z is a zig-zag chain. Then

$$TI(Y_1) - TI(X_1) = 4\varphi_{24} + 2\varphi_{44} - 2\varphi_{23} - 4\varphi_{34}$$

Proof. Let M_1 be the set of edges in bold of X_1 and N_1 the set of edges in bold in Y_1 as shown in Figure 1. Then there exist a one-to-one correspondence between the set of edges $E(X_1)\backslash M_1$ and $E(Y_1)\backslash N_1$, in such a way that the degrees of the end vertices of every edge in $E(X_1)\backslash M_1$ are equal to those of the correspondent edge in $E(Y_1)\backslash N_1$. Since M_1 consists of two 23-edges and four 34-edges, and N_1 consists of four 24-edges and two 44-edges, then

$$\begin{aligned} TI(Y_1) - TI(X_1) &= (4\varphi_{24} + 2\varphi_{44}) - (2\varphi_{23} + 4\varphi_{34}) \\ &= 4\varphi_{24} + 2\varphi_{44} - 2\varphi_{23} - 4\varphi_{34} \end{aligned}$$

■

Our second operation is shown in Figure 2.

Lemma 2.2 *Let TI be a topological index induced by the numbers $\{\varphi_{ij}\}$. Consider the angularizing operation 2 shown in Figure 2, where X is a polyomino chain and Z is a zig-zag chain. Then*

$$TI(Y_2) - TI(X_2) = 4\varphi_{24} + \varphi_{44} - 2\varphi_{23} - 2\varphi_{34} - \varphi_{33}$$

Proof. Let M_2 be the set of edges in bold of X_2 and N_2 the set of edges in bold in Y_2 as shown in Figure 2. Then there exist a one-to-one correspondence between the set of edges $E(X_2)\backslash M_2$ and $E(Y_2)\backslash N_2$, in such a way that the degrees of the end vertices of every edge in $E(X_2)\backslash M_2$ are equal to those of the correspondent edge in $E(Y_2)\backslash N_2$. Since M_2 consists of two 23-edges, two 34-edges, one 33-edge and one 44-edge, and N_2 consists of four 24-edges and two 44-edges, then

$$\begin{aligned} TI(Y_2) - TI(X_2) &= (4\varphi_{24} + 2\varphi_{44}) - (2\varphi_{23} + 2\varphi_{34} + \varphi_{33} + \varphi_{44}) \\ &= 4\varphi_{24} + \varphi_{44} - 2\varphi_{23} - 2\varphi_{34} - \varphi_{33} \end{aligned}$$

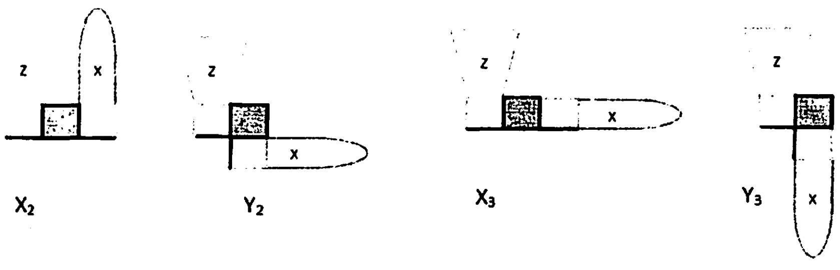

Figure 2: Angularizing operations 2 and 3.

■

The angularizing operation 3 is shown in Figure 2.

Lemma 2.3 *Let TI be a topological index induced by the numbers $\{\varphi_{ij}\}$. Consider the angularizing operation 3 shown in Figure 2, where X is a polyomino chain and Z is a zig-zag chain. Then*

$$TI(Y_3) - TI(X_3) = 2\varphi_{24} + \varphi_{44} - 3\varphi_{33}$$

Proof. Let M_3 be the set of edges in bold of X_3 and N_3 the set of edges in bold in Y_3 as shown in Figure 2. Then there exist a one-to-one correspondence between the set of edges $E(X_3)\backslash M_3$ and $E(Y_3)\backslash N_3$, in such a way that the degrees of the end vertices of every edge in $E(X_3)\backslash M_3$ are equal to those of the correspondent edge in $E(Y_3)\backslash N_3$. Since M_3 consists of three 33-edges, two 34-edges and one 23-edge, and N_2 consists of two 24-edges, one 23-edge, two 34-edges and one 44-edge, then

$$\begin{aligned} TI(Y_3) - TI(X_3) &= (2\varphi_{24} + \varphi_{23} + 2\varphi_{34} + \varphi_{44}) - (3\varphi_{33} + 2\varphi_{34} + \varphi_{23}) \\ &= 2\varphi_{24} + \varphi_{44} - 3\varphi_{33} \end{aligned}$$

■

Finally we will need two angularizing operations when the linear square is adjacent to a terminal square of the polyomino chain.

Lemma 2.4 *Let TI be a topological index induced by the numbers $\{\varphi_{ij}\}$. Consider the angularizing operations 4 and 5 shown in Figure 3, where X is a polyomino chain. Then*

$$TI(Y_4) - TI(X_4) = 3\varphi_{24} - \varphi_{23} - \varphi_{34} + \varphi_{44} - 2\varphi_{33}$$

and

$$TI(Y_5) - TI(X_5) = \varphi_{23} + 3\varphi_{34} + \varphi_{24} - 5\varphi_{33}$$

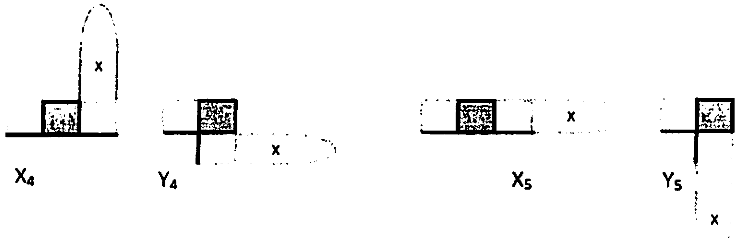

Figure 3: Angularizing operations 4 and 5.

Proof. This was shown in [15]. ■

We illustrate in our next example how to transform a polyomino chain into a zig-zag chain in a finite number of steps, using the angularizing operations defined above.

Example 2.5 *In Figure 4 we show how to construct a sequence of polyomino chains using operations 1-5 given above to reach the zig-zag chain. In each step we apply the operation over the first linear square that appears in the chain, represented with a shadowed square.*

Now we show that the zig-zag chain has extremal TI-value among all polyomino chains with a fixed number of squares.

Theorem 2.6 *Let TI be a topological index induced by the numbers $\{\varphi_{ij}\}$.*

1. *If*

$$\begin{cases} 4\varphi_{24} + 2\varphi_{44} - 2\varphi_{23} - 4\varphi_{34} \geq 0 \\ 4\varphi_{24} + \varphi_{44} - 2\varphi_{23} - 2\varphi_{34} - \varphi_{33} \geq 0 \\ 2\varphi_{24} + \varphi_{44} - 3\varphi_{33} \geq 0 \\ 3\varphi_{24} - \varphi_{23} - \varphi_{34} + \varphi_{44} - 2\varphi_{33} \geq 0 \\ \varphi_{23} + 3\varphi_{34} + \varphi_{24} - 5\varphi_{33} \geq 0 \end{cases}$$

then Z_n has maximal TI-value among all polyomino chains of n squares.

2. *If*

$$\begin{cases} 4\varphi_{24} + 2\varphi_{44} - 2\varphi_{23} - 4\varphi_{34} \leq 0 \\ 4\varphi_{24} + \varphi_{44} - 2\varphi_{23} - 2\varphi_{34} - \varphi_{33} \leq 0 \\ 2\varphi_{24} + \varphi_{44} - 3\varphi_{33} \leq 0 \\ 3\varphi_{24} - \varphi_{23} - \varphi_{34} + \varphi_{44} - 2\varphi_{33} \leq 0 \\ \varphi_{23} + 3\varphi_{34} + \varphi_{24} - 5\varphi_{33} \leq 0 \end{cases}$$

then Z_n has minimal TI-value among all polyomino chains of n squares.

Proof. 1. We will show that the TI-value of a polyomino chain P with n squares is less than or equal to the TI-value of Z_n. We use induction on the number of linear squares l of the polyomino chain P. If $l = 0$ then $P = Z_n$ and we are done. Assume that the result holds for $l \geq 0$ and let P be a polyomino chain with $l + 1$ linear squares. Choose the first linear square that appears in P. Then P is of the form X_i for some $i = 1, 2, 3, 4$ or 5 in Figures 1-3. Then by our hypothesis $TI(Y_i) - TI(X_i) \geq 0$ and clearly Y_i has l linear squares. Then by our induction hypothesis $TI(Y_i) \leq TI(Z_n)$ and so

$$TI(P) = TI(X_i) \leq TI(Y_i) \leq TI(Z_n)$$

2. The proof is similar. ■

We now apply Theorem 2.6 to concrete topological indices TI.

Corollary 2.7 *Among all polyomino chains with n squares, the Randić index, the sum-connectivity index, the harmonic index and the geometric-arithmetic index attain the minimal value in Z_n, and the first Zagreb, second Zagreb and the atom-bond-connectivity index attain the maximal value in Z_n.*

Proof. The values of

$$4\varphi_{24} + 2\varphi_{44} - 2\varphi_{23} - 4\varphi_{34} \tag{2}$$

$$4\varphi_{24} + \varphi_{44} - 2\varphi_{23} - 2\varphi_{34} - \varphi_{33} \tag{3}$$

$$2\varphi_{24} + \varphi_{44} - 3\varphi_{33} \tag{4}$$

$$3\varphi_{24} - \varphi_{23} - \varphi_{34} + \varphi_{44} - 2\varphi_{33} \tag{5}$$

$$\varphi_{23} + 3\varphi_{34} + \varphi_{24} - 5\varphi_{33} \tag{6}$$

are calculated in the following table:

	(2)	(3)	(4)	(5)	(6)
Randić	−.05	−.06	−.04	−.05	−.03
Sum-connectivity	−.06	−.07	−.05	−.06	−.05
Harmonic	−.10	−.12	−.08	−.10	−.07
Geometric-Arithmetic	−.14	−.16	−.11	−.14	−.10
First Zagreb	2	2	2	2	2
Second Zagreb	4	3	5	4	5
Atom-bond-connectivity	.05	.06	.02	.04	.01

As we can see, the Randić index, the sum-connectivity index, the harmonic index and the geometric-arithmetic index satisfy the conditions in part 2 of Theorem 2.6. Hence the minimal value for these indices is attained in Z_n. On the other hand, the first Zagreb, the second Zagreb and the atom-bond-connectivity index

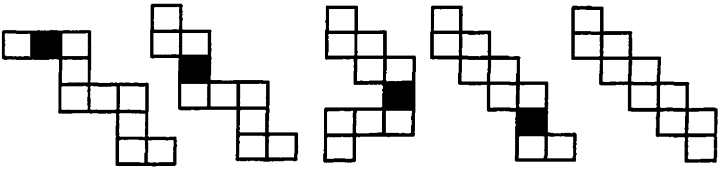

Figure 4: Sequence of polyomino chains ending in the zig-zag chain

satisfy part 1 of Theorem 2.6, which implies that the maximal value is attained in Z_n for these indices. ∎

We note that the values of the augmented Zagreb index are given by

Augmented Zagreb	-1.37	-4.07	$.79$	-1.64	$.51$

Consequently, we cannot conclude that the zig-zag chain is an extremal value for the augmented Zagreb index.

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