Applied Mathematical Sciences, Vol. 10, 2016, no. 10, 487 - 501
HIKARI Ltd, www.m-hikari.com
http://dx.doi.org/10.12988/ams.2016.59613

Extremal Values of VDB Topological Indices over Catacondensed Polyomino Systems

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Abstract

A VDB topological index is defined as

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

where G is a graph with n vertices and m_{ij} is the number of ij-edges. We study T over the set of catacondensed polyomino systems. Specifically, we introduce two unbranching operations and show that under certain conditions on $\{\varphi_{ij}\}$, T is monotone with respect to these operations. We apply these results to find extremal values of T over the set of catacondensed polyomino systems.

Mathematics Subject Classification: 05C12, 05C05

Keywords: VDB indices; Catacondensed polyomino systems; Polyomino chains; Extreme values

1 Introduction

A great variety of vertex-degree-based topological indices (VDB indices for short) have been considered in the mathematico-chemical literature [8]. Given nonnegative real numbers $\{\varphi_{ij}\}$ for every $1 \le i \le j \le n-1$, they are of the form

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

where G is a graph with n vertices and m_{ij} is the number of edges of G connecting a vertex of degree i with a vertex of degree j. Several important VDB topological indices are induced by the different choices of the numbers $\{\varphi_{ij}\}$. For example, the Randić index is obtained from $\varphi_{ij} = \frac{1}{\sqrt{ij}}$ [13], the sum-connectivity index from $\varphi_{ij} = \frac{1}{\sqrt{i+j}}$ [21], the harmonic index from $\varphi_{ij} = \frac{2}{i+j}$ [20], the geometric-arithmetic from $\varphi_{ij} = \frac{2\sqrt{ij}}{i+j}$ [14], the first Zagreb index from $\varphi_{ij} = i + j$ [10], the second Zagreb index from $\varphi_{ij} = ij$ [10], the atom-bond-connectivity index from $\varphi_{ij} = \sqrt{\frac{i+j-2}{ij}}$ [6] and the augmented Zagreb index from $\varphi_{ij} = \left(\frac{ij}{i+j-2}\right)^3$ [7].

In this paper we study T as in (1) over the set of catacondensed polyomino systems. Recall that a polyomino system [9] 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 catacondensed polyomino system is a polyomino system whose inner dual graph is a tree (see Figure 1). Note that the maximal degree of the inner dual tree is 4. A branching square of a catacondensed polyomino system is any square whose corresponding vertex in the inner dual tree has degree 3 or 4 (shadow squares in Figure 1).

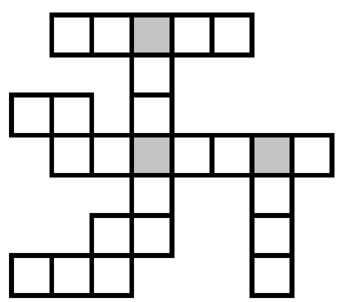

Figure 1: Catacondensed polyomino system.

A polyomino chain is a polyomino system whose inner dual graph is a path. It means that a polyomino chain is a catacondensed polyomino system with no branching squares. 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, the linear chain L_n is a polyomino chain with exactly one segment (of length n) and the zig-zag chain Z_n is a polyomino chain in which every segment has length 2 (see Figure

2).

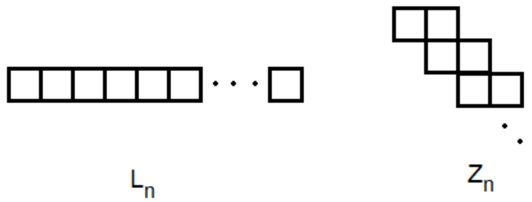

Figure 2: Linear chain L_n and Zig-zag chain Z_n.

The problem of finding extremal polyomino chains with respect to vertex-degree-based topological indices has recently attracted much attention in the literature. For instance, Yang et al. ([17],[18]) and Yarahmadi et al. [16] find formulas for the Randić index, the sum-connectivity index and the Zagreb indices of polyomino chains and deduce the extremal values; more recently, An and Xiong [2] generalized some of the previous results to general Randić indices and Deng et al. [5] found formulas for the harmonic indices and deduced the extremal values. Other results can be found in ([15],[19]).

In ([11], [12]) Rada introduced several transformations of polyomino chains and gave conditions on the numbers $\{\varphi_{ij}\}$ that assure that the linear chain or the zig-zag chain are extremal values of the induced VDB topological index T. In [4] the so called linear and angular transformations were completed and a new extremal polyomino chain with respect to VDB indices was introduced. Namely, the zig-zag chain of segments of length 3, denoted by Z_n^3, has minimal atom-bond-connectivity index among all polyomino chains with n squares.

In [1] Ali et al. established a general expression for calculating the VDB indices of polyomino chains, recovered the previous results about extremal values of different VDB indices and found the extremal polyomino chains with respect to augmented Zagreb index.

On the other hand, the problem of finding extremal catacondensed polyomino systems with respect to VDB topological indices has received less attention. In [3] Chen at el. prove that the polyomino chain Z_n has the maximal value with respect to the atom-bond-connectivity index.

In our study we introduce two unbranching operations over catacondensed polyomino systems and show that under certain conditions on the numbers $\{\varphi_{ij}\}$, the topological index T defined as in (1) is monotone with respect to these operations. Then we apply these results to find extremal values of T over the set of catacondensed polyomino systems.

2 Unbranching operations on catacondensed polyomino systems.

$\mathcal{CP}_n$ will denote the set of all catacondensed polyomino systems with n squares. If P is a catacondensed polyomino system, then we denote by $|P|$ the number of squares P has. Let $b_4(P)$ be the number of branching squares of degree 4 and $b_3(P)$ the number of branching squares of degree 3 P has. Then $b(P) = b_4(P) + b_3(P)$ is the total number of branching squares in P.

$\mathcal{P}_n$ will denote the set of all polyomino chains with n squares. Note that $\mathcal{P}_n$ is properly contained in $\mathcal{CP}_n$, since a polyomino chain is a catacondensed polyomino system with no branching squares.

In our first result we prove that under certain conditions, from any catacondensed polyomino system P with $b_4(P) > 0$ one can construct a catacondensed polyomino system Q with $b_4(Q) = b_4(P) - 1$ and such that $T(P) \leq T(Q)$.

For a vertex u of the catacondensed polyomino system, we denote by d_u the degree of this vertex. Note that $d_u \in \{2, 3, 4\}$. In the proof of the next lemma we will distinguish vertices u, v, w, x, y, z of the catacondensed polyomino system with degrees that satisfy the following conditions:

C1: $(d_u, d_v) \in \{(2,2); (3,3); (3,4); (4,3); (4,4)\}$.

C2: If $d_u = 4$ then $d_w \in \{2; 3\}$, otherwise $d_w \in \{2; 3; 4\}$.

C3: If $d_v = 4$ then $d_x \in \{2; 3\}$, otherwise $d_x \in \{2; 3; 4\}$.

C4: $(d_y, d_z) \in \{(3,3); (3,4); (4,3); (4,4)\}$.

Next we define two functions of the degrees of the vertices u, v, w, x, y, z. Let D_1 be the set of the 3-tuplas (d_u, d_v, d_w) that satisfy conditions C1 and C2 and D_2 be the set of the 6-tuplas $(d_u, d_v, d_w, d_x, d_y, d_z)$ that satisfy conditions C1, C2, C3 and C4. Over D_1 and D_2 we define the functions F_1 and F_2 respectively as follows:

$$\begin{aligned} F_1(d_u, d_v, d_w) &= (\varphi_{4d_u} - \varphi_{3d_u}) + (\varphi_{4d_v} - \varphi_{3d_v}) + (\varphi_{4d_w} - \varphi_{3d_w}) \\ F_2(d_u, d_v, d_w, d_x, d_y, d_z) &= F_1(d_u, d_v, d_w) + \\ &\quad + (\varphi_{4d_x} - \varphi_{3d_x}) + \left(\varphi_{2d_y} - \varphi_{3d_y}\right) + (\varphi_{2d_z} - \varphi_{3d_z}) \end{aligned}$$

The following numbers will be used in the sequel

$$\alpha_1 = \varphi_{22} + 2\varphi_{24} - 3\varphi_{33} - 3\varphi_{34} + 3\varphi_{44} + \max_{D_1} F_1(d_u, d_v, d_w) \quad (2)$$
$$\beta_1 = \varphi_{22} + 2\varphi_{24} - 3\varphi_{33} - 3\varphi_{34} + 3\varphi_{44} + \min_{D_1} F_1(d_u, d_v, d_w) \quad (3)$$
$$\alpha_2 = \varphi_{22} + 2\varphi_{23} - 5\varphi_{33} - \varphi_{34} + 3\varphi_{44} + \max_{D_1} F_1(d_u, d_v, d_w) \quad (4)$$
$$\beta_2 = \varphi_{22} + 2\varphi_{23} - 5\varphi_{33} - \varphi_{34} + 3\varphi_{44} + \min_{D_1} F_1(d_u, d_v, d_w) \quad (5)$$
$$\alpha_3 = \varphi_{22} - 2\varphi_{33} - 2\varphi_{34} + 3\varphi_{44} + \max_{D_2} F_2(d_u, d_v, d_w, d_x, d_y, d_z) \quad (6)$$
$$\beta_3 = \varphi_{22} - 2\varphi_{33} - 2\varphi_{34} + 3\varphi_{44} + \min_{D_2} F_2(d_u, d_v, d_w, d_x, d_y, d_z) \quad (7)$$

Lemma 1 *Let $P \in \mathcal{CP}_n$ with $b_4(P) > 0$ and T be a VDB topological index defined as in (1) .*

1. *If $\alpha_i \leq 0$ for $i = 1, \ldots, 3$ then there exists a catacondensed polyomino system Q with $b_4(Q) = b_4(P) - 1$ such that $T(P) \leq T(Q)$.*
2. *If $\beta_i \geq 0$ for $i = 1, \ldots, 3$ then there exists a catacondensed polyomino system Q with $b_4(Q) = b_4(P) - 1$ such that $T(P) \geq T(Q)$.*

Proof. Let $P \in \mathcal{CP}_n$ such that $b_4(P) > 0$. The form of P is depicted in Figure 3 where A, B, C and D are catacondensed polyomino subsystems. We have to consider three cases:

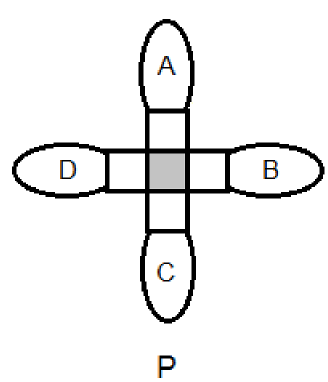

Figure 3: Catacondensed polyomino system with $b_4 > 0$.

Case 1: $|B| = 0$. Let $Q \in \mathcal{CP}_n$ obtained from P as depicted in Figure 4. Note that D_1 is the set of the possible values of the degrees of the vertices u, v, w.

If we denote by M_P (resp. M_Q) the set of edges in bold of P (resp. Q) then there exists a one-to-one correspondence between the set of edges $E(P) \backslash M_P$

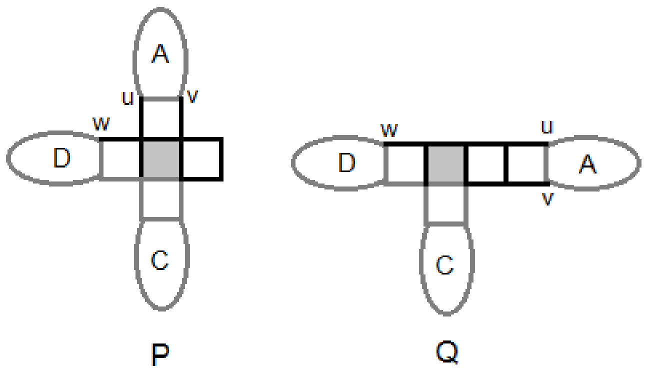

Figure 4: Catacondensed polyomino system used in the proof of the Case 1 of Lemma 1 .

and $E(Q)\setminus M_Q$, in such a way that the degrees of the end vertices of every edge in $E(P)\setminus M_P$ are equal to those of the corresponding edge in $E(Q)\setminus M_Q$. Since M_P consists of one 22-edge, two 24-edges, three 44-edges, one $4d_u$-edge, one $4d_v$-edge and one $4d_w$-edge, and M_Q consists of three 33-edges, three 34-edges, one $3d_u$-edge, one $3d_v$-edge and one $3d_w$-edge, then

$$\begin{aligned} T(P)-T(Q) &= (\varphi_{22}+2\varphi_{24}+3\varphi_{44}+\varphi_{4d_u}+\varphi_{4d_v}+\varphi_{4d_w})- \\ &\quad -(3\varphi_{33}+3\varphi_{34}+\varphi_{3d_u}+\varphi_{3d_v}+\varphi_{3d_w}) \\ &= \varphi_{22}+2\varphi_{24}-3\varphi_{33}-3\varphi_{34}+3\varphi_{44}+F_1(d_u,d_v,d_w) \end{aligned}$$

From equations (2) and (3) we obtain that

$$\beta_1 \leq T(P)-T(Q) \leq \alpha_1. \tag{8}$$

Case 2: $|B|=1$. Let $Q\in\mathcal{CP}_n$ obtained from P as depicted in Figure 5. Note that D_1 is the set of the possible values of the degrees of the vertices u,v,w.

As in the previous case, let M_P (resp. M_Q) be the set of edges in bold of P (resp. Q). Since M_P consists of one 22-edge, two 23-edges, one 34-edge, three 44-edges, one $4d_u$-edge, one $4d_v$-edge and one $4d_w$-edge, and M_Q consists of five 33-edges, two 34-edges, one $3d_u$-edge, one $3d_v$-edge and one $3d_w$-edge, then

$$\begin{aligned} T(P)-T(Q) &= (\varphi_{22}+2\varphi_{23}+\varphi_{34}+3\varphi_{44}+\varphi_{4d_u}+\varphi_{4d_v}+\varphi_{4d_w})- \\ &\quad -(5\varphi_{33}+2\varphi_{34}+\varphi_{3d_u}+\varphi_{3d_v}+\varphi_{3d_w}) \\ &= \varphi_{22}+2\varphi_{23}-5\varphi_{33}-\varphi_{34}+3\varphi_{44}+F_1(d_u,d_v,d_w) \end{aligned}$$

From equations (4) and (5) we obtain that

$$\beta_2 \leq T(P)-T(Q) \leq \alpha_2. \tag{9}$$

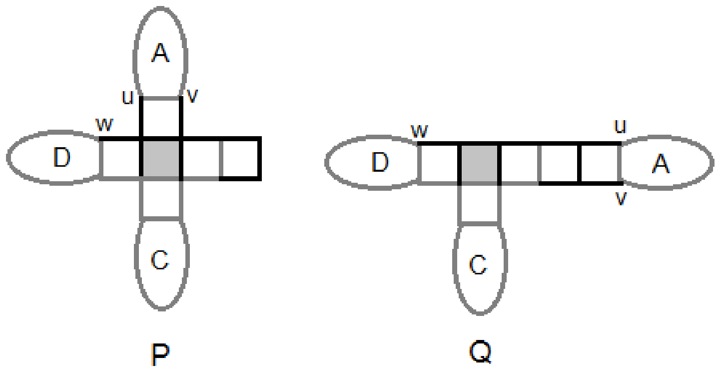

Figure 5: Catacondensed polyomino system used in the proof of the Case 2 of Lemma 1 .

Case 3: $|B| > 1$. Let $Q \in \mathcal{CP}_n$ obtained from P as depicted in Figure 6. Note that D_2 is the set of the possible values of the degrees of the vertices u, v, w, x, y, z.

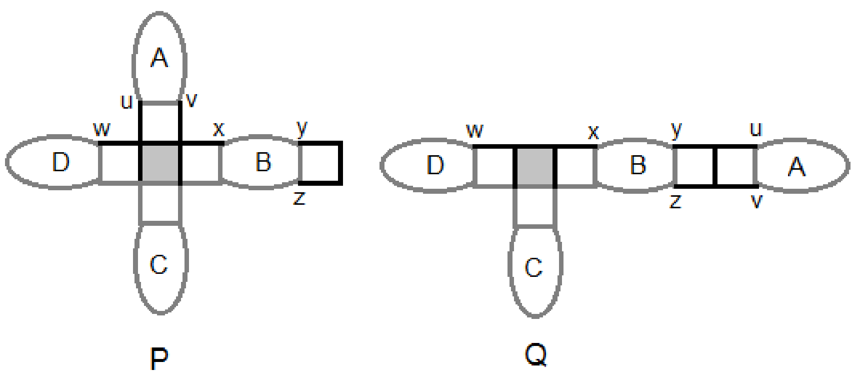

Figure 6: Catacondensed polyomino system used in the proof of the Case 3 of Lemma 1 .

If M_P (resp. M_Q) is the set of edges in bold of P (resp. Q) then M_P consists of one 22-edge, three 44-edges, one $4d_u$-edge, one $4d_v$-edge, one $4d_w$-edge, one $4d_x$-edge, one $2d_y$-edge and one $2d_z$-edge, and M_Q consists of two 33-edges, two 34-edges, one $3d_u$-edge, one $3d_v$-edge, one $3d_w$-edge, one $3d_x$-edge, one $3d_y$-edge and one $3d_z$-edge. Then

$$\begin{aligned} T(P) - T(Q) &= \left(\varphi_{22} + 3\varphi_{44} + \varphi_{4d_u} + \varphi_{4d_v} + \varphi_{4d_w} + \varphi_{4d_x} + \varphi_{2d_y} + \varphi_{2d_z}\right) - \\ &\quad - \left(2\varphi_{33} + 2\varphi_{34} + \varphi_{3d_u} + \varphi_{3d_v} + \varphi_{3d_w} + \varphi_{3d_x} + \varphi_{3d_y} + \varphi_{3d_z}\right) \\ &= \varphi_{22} - 2\varphi_{33} - 2\varphi_{34} + 3\varphi_{44} + F_2\left(d_u, d_v, d_w, d_x, d_x, d_z\right) \end{aligned}$$

From equations (6) and (7) we obtain that

$$\beta_3 \leq T(P) - T(Q) \leq \alpha_3. \tag{10}$$

In each one of the three cases, the polyomino system Q is such that $b_4(Q) = b_4(P) - 1$. The proof of both parts of the lemma is obtained from inequalities (8), (9) and (10). ■

In our next result we prove that under certain conditions, from any catacondensed polyomino system P with $b_3(P) > 0$ one can construct a catacondensed polyomino system Q with $b_3(Q) = b_3(P) - 1$ and such that $T(P) \leq T(Q)$. In addition to the vertices u, v, w, x, y, z with degrees that satisfy conditions C1, C2, C3 and C4, we will distinguish two more vertices s, t of the catacondensed polyomino system with degrees that satisfy the following conditions:

C5: $d_s \in \{3, 4\}$.

C6: $d_t \in \{3, 4\}$.

Next we define two more functions of the degrees of the vertices u, v, w, x, y, z, s, t. Let D_3 be the set of the 4-tuplas (d_u, d_v, d_w, d_s) that satisfy conditions C1, C2 and C5 and D_4 be the set of the 8-tuplas $(d_u, d_v, d_w, d_x, d_y, d_z, d_s, d_t)$ that satisfy conditions C1, C2, C3, C4, C5 and C6. Over D_3 and D_4 we define the functions F_3 and F_4 respectively as follows:

$$\begin{aligned} F_3(d_u, d_v, d_w, d_s) &= F_1(d_u, d_v, d_w) + (\varphi_{4d_s} - \varphi_{3d_s}) \\ F_4(d_u, d_v, d_w, d_x, d_y, d_z, d_s, d_t) &= F_2(d_u, d_v, d_w, d_x, d_y, d_z) + (\varphi_{4d_s} - \varphi_{3d_s}) + \\ &\quad + (\varphi_{4d_t} - \varphi_{3d_s}) \end{aligned}$$

The following numbers will be used in the sequel

$$\alpha_4 = \varphi_{22} + \varphi_{23} + \varphi_{24} - 5\varphi_{33} + \varphi_{34} + \varphi_{44} + \max_{D_3} F_3(d_u, d_v, d_w, d_s) \tag{11}$$

$$\beta_4 = \varphi_{22} + \varphi_{23} + \varphi_{24} - 5\varphi_{33} - \varphi_{34} + \varphi_{44} + \min_{D_3} F_3(d_u, d_v, d_w, d_s) \tag{12}$$

$$\alpha_5 = \varphi_{22} + 2\varphi_{23} - 6\varphi_{33} + 2\varphi_{34} + \varphi_{44} + \max_{D_3} F_3(d_u, d_v, d_w, d_s) \tag{13}$$

$$\beta_5 = \varphi_{22} + 2\varphi_{23} - 6\varphi_{33} + 2\varphi_{34} + \varphi_{44} + \min_{D_3} F_3(d_u, d_v, d_w, d_s) \tag{14}$$

$$\alpha_6 = \varphi_{22} + 2\varphi_{24} - 3\varphi_{33} - 2\varphi_{34} + 2\varphi_{44} + \max_{D_3} F_3(d_u, d_v, d_w, d_s) \tag{15}$$

$$\beta_6 = \varphi_{22} + 2\varphi_{24} - 3\varphi_{33} - 2\varphi_{34} + 2\varphi_{44} + \min_{D_3} F_3(d_u, d_v, d_w, d_s) \tag{16}$$

$$\alpha_7 = \varphi_{22} - 2\varphi_{33} + \varphi_{44} + \max_{D_4} F_4(d_u, d_v, d_w, d_x, d_y, d_z, d_s, d_t) \tag{17}$$

$$\beta_7 = \varphi_{22} - 2\varphi_{33} + \varphi_{44} + \min_{D_4} F_4(d_u, d_v, d_w, d_x, d_y, d_z, d_s, d_t) \tag{18}$$

Lemma 2 *Let $P \in \mathcal{CP}_n$ with $b_3(P) > 0$ and T be a VDB topological index defined as in (1) .*

1. *If $\alpha_i \leq 0$ for $i = 4, \dots, 7$ then there exists a catacondensed polyomino system Q with $b_3(Q) = b_3(P) - 1$ such that $T(P) \leq T(Q)$.*
2. *If $\beta_i \geq 0$ for $i = 4, \dots, 7$ then there exists a catacondensed polyomino system Q with $b_3(Q) = b_3(P) - 1$ such that $T(P) \geq T(Q)$.*

Proof. Let P be a catacondensed polyomino system with n squares such that $b_3(P) > 0$. The form of P is depicted in Figure 7 where A, B and C are catacondensed polyomino subsystems. We have to consider four cases:

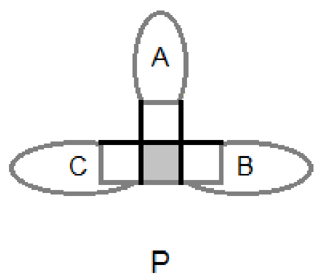

Figure 7: Catacondensed polyomino system with $b_3 > 0$.

Case 1: $|B| = 0$. Let $Q \in \mathcal{CP}_n$ obtained from P as depicted in Figure 8. Note that D_3 is the set of the possible values of the degrees of the vertices u, v, w, s.

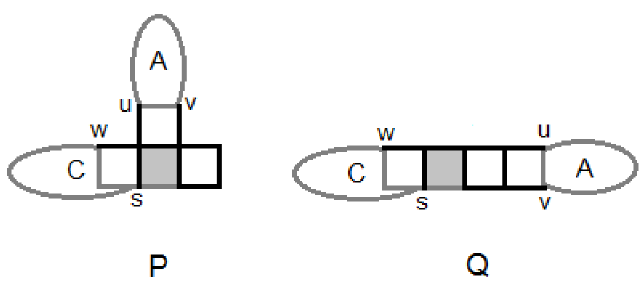

Figure 8: Catacondensed polyomino system used in the proof of the Case 1 of Lemma 2 .

If M_P (resp. M_Q) is the set of edges in bold of P (resp. Q), since M_P consists of one 22-edge, one 23-edge, one 24-edge, one 34-edge, one 44-edge, one $4d_u$-edge, one $4d_v$-edge, one $4d_w$-edge and one $4d_s$-edge, and M_Q consists of five 33-edges, one $3d_u$-edge, one $3d_v$-edge, one $3d_w$-edge and one $3d_s$-edge, then

$$\begin{aligned} T(P)-T(Q) &= (\varphi_{22}+\varphi_{23}+\varphi_{24}+\varphi_{34}+\varphi_{44}+\varphi_{4d_u}+\varphi_{4d_v}+\varphi_{4d_w}+\varphi_{4d_s})- \\ &\quad -(5\varphi_{33}+\varphi_{3d_u}+\varphi_{3d_v}+\varphi_{3d_w}+\varphi_{3d_s}) \\ &= \varphi_{22}+\varphi_{23}+\varphi_{24}-5\varphi_{33}+\varphi_{34}+\varphi_{44}+F_3(d_u,d_v,d_w,d_s) \end{aligned}$$

From equations (11) and (12) we obtain that

$$\beta_4 \leq T(P)-T(Q) \leq \alpha_4. \tag{19}$$

Case 2: $|B|=1$ and P is of the form illustrated in Figure 9. Let $Q \in \mathcal{CP}_n$ obtained from P as depicted in Figure 9. Note that D_3 is the set of the possible values of the degrees of the vertices u,v,w,s.

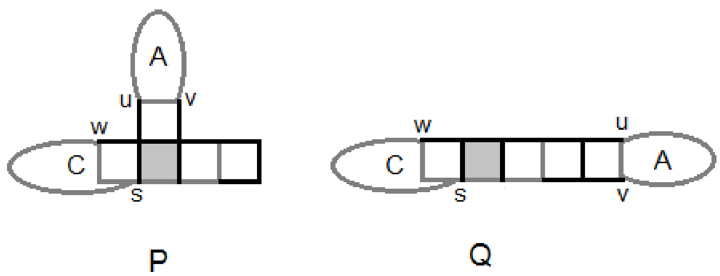

Figure 9: Catacondensed polyomino system used in the proof of the Case 2 of Lemma 2 .

If M_P (resp. M_Q) is the set of edges in bold of P (resp. Q), since M_P consists of one 22-edge, two 23-edges, two 34-edges, one 44-edge, one $4d_u$-edge, one $4d_v$-edge, one $4d_w$-edge and one $4d_s$-edge, and M_Q consists of six 33-edges, one $3d_u$-edge, one $3d_v$-edge, one $3d_w$-edge and one $3d_s$-edge, then

$$\begin{aligned} T(P)-T(Q) &= (\varphi_{22}+2\varphi_{23}+2\varphi_{34}+\varphi_{44}+\varphi_{4d_u}+\varphi_{4d_v}+\varphi_{4d_w}+\varphi_{4d_s})- \\ &\quad -(6\varphi_{33}+\varphi_{3d_u}+\varphi_{3d_v}+\varphi_{3d_w}+\varphi_{3d_s}) \\ &= \varphi_{22}+2\varphi_{23}-6\varphi_{33}+2\varphi_{34}+\varphi_{44}+F_3(d_u,d_v,d_w,d_s) \end{aligned}$$

From equations (13) and (14) we obtain that

$$\beta_5 \leq T(P)-T(Q) \leq \alpha_5. \tag{20}$$

Case 3: $|B|=1$ and P is of the form illustrated in Figure 10. Let $Q \in \mathcal{CP}_n$ obtained from P as depicted in Figure 10. Note that D_3 is the set of the possible values of the degrees of the vertices u,v,w,s.

If M_P (resp. M_Q) is the set of edges in bold of P (resp. Q), since M_P consists of one 22-edge, one 23-edge, two 24-edges, two 44-edges, one $4d_u$-edge,

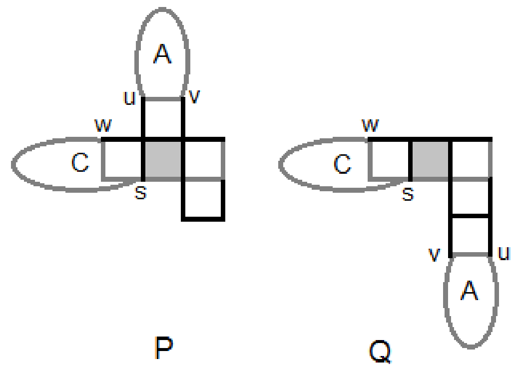

Figure 10: Catacondensed polyomino system used in the proof of the Case 3 of Lemma 2 .

one $4d_v$-edge, one $4d_w$-edge and one $4d_s$-edge, and M_Q consists of one 23-edge, three 33-edges, two 34-edges, one $3d_u$-edge, one $3d_v$-edge, one $3d_w$-edge and one $3d_s$-edge, then

$$\begin{aligned} T(P) - T(Q) &= (\varphi_{22} + \varphi_{23} + 2\varphi_{24} + 2\varphi_{44} + \varphi_{4d_u} + \varphi_{4d_v} + \varphi_{4d_w} + \varphi_{4d_s}) - \\ &\quad - (\varphi_{23} + 3\varphi_{33} + 2\varphi_{34} + \varphi_{3d_u} + \varphi_{3d_v} + \varphi_{3d_w} + \varphi_{3d_s}) \\ &= \varphi_{22} + 2\varphi_{24} - 3\varphi_{33} - 2\varphi_{34} + 2\varphi_{44} + F_3(d_u, d_v, d_w, d_s) \end{aligned}$$

From equations (15) and (16) we obtain that

$$\beta_6 \leq T(P) - T(Q) \leq \alpha_6. \tag{21}$$

Case 4: $|B| > 1$. Let $Q \in \mathcal{CP}_n$ obtained from P as depicted in Figure 11. Note that D_4 is the set of the possible values of the degrees of the vertices u, v, w, x, y, z, s, t.

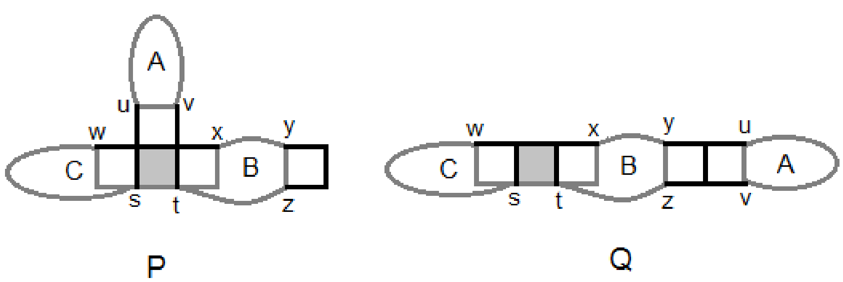

Figure 11: Catacondensed polyomino system used in the proof of the Case 4 of Lemma 2 .

If M_P (resp. M_Q) is the set of edges in bold of P (resp. Q), since M_P consists of one 22-edge, one 44-edge, one $4d_u$-edge, one $4d_v$-edge, one $4d_w$-edge, one $4d_x$-edge, one $2d_y$-edge, one $2d_z$-edge, one $4d_s$-edge and one $4d_t$-edge, and M_Q consists of two 33-edges, one $3d_u$-edge, one $3d_v$-edge, one $3d_w$-edge , one $3d_x$-edge, one $3d_y$-edge, one $3d_z$-edge, one $3d_s$-edge and one $3d_t$-edge, then

$$\begin{aligned} T(P) - T(Q) &= \left(\varphi_{22} + \varphi_{44} + \varphi_{4d_u} + \varphi_{4d_v} + \varphi_{4d_w} + \varphi_{4d_x} + \varphi_{2d_y} + \varphi_{2d_z} + \varphi_{4d_s} + \varphi_{4d_t}\right) - \\ &\quad - \left(2\varphi_{33} + \varphi_{3d_u} + \varphi_{3d_v} + \varphi_{3d_w} + \varphi_{3d_x} + \varphi_{3d_y} + \varphi_{3d_z} + \varphi_{3d_s} + \varphi_{3d_t}\right) \\ &= \varphi_{22} - 2\varphi_{33} + \varphi_{44} + F_4(d_u, d_v, d_w, d_x, d_y, d_t, d_s, d_t) \end{aligned}$$

From equations (17) and (18) we obtain that

$$\beta_7 \leq T(P) - T(Q) \leq \alpha_7. \tag{22}$$

In each one of the four cases, the polyomino system Q is such that $b_3(Q) = b_3(P) - 1$. The proof of both parts of the Lemma is obtained from inequalities (19), (20), (21) and (22). ■

3 Extremal values of VDB topological indices over catacondensed polyomino systems.

Our main result is the following

Theorem 3 *Let T be a VDB topological index defined as in (1) .*

1. *If $\alpha_i \leq 0$ for $i = 1, \ldots, 7$ then the maximal catacondensed polyomino system with n squares with respect to VDB index T is a polyomino chain.*

2. *If $\beta_i \geq 0$ for $i = 1, \ldots, 7$ then the minimal catacondensed polyomino system with n squares with respect to VDB index T is a polyomino chain.*

Proof. Part 1. Let P be a catacondensed polyomino system with n squares and $b_4(P) > 0$, applying repeatedly Lemma 1 we obtain a catacondensed polyomino system P' such that $b_4(P') = 0$ and $T(P) \leq T(P')$. Now if $b_3(P') = 0$ then P' has no branching squares. It means that P' is a polyomino chain and we are done. If $b_3(P') > 0$ then applying repeatedly Lemma 2 we obtain a catacondensed polyomino system Q such that $b(Q) = b_4(Q) + b_3(Q) = 0$ and $T(P) \leq T(Q)$. Since Q is a polyomino chain we are done.
The part 2 of the Theorem is proved similarly. ■

Applying Theorem 3 to the the Randić index, the sum-connectivity index, the geometric-arithmetic index, the harmonic index, the first Zagreb index and the second Zagreb index and since we know the extremal polyomino chains over $\mathcal{P}_n$ with respect to these indices we obtain the following result:

Corollary 4 *Among all catacondensed polyomino systems with n squares, the Randić index, the sum-connectivity index, the geometric-arithmetic index and the harmonic index attain the maximal value in the linear polyomino chain L_n. The first Zagreb index and the second Zagreb index attain the minimal value in the linear polyomino chain L_n.*

Proof. The values of α_i and β_i for $i = 1, \ldots, 7$ are shown in Table 1. As we can see, the Randić index, the sum-connectivity index, the geometric-arithmetic index and the harmonic index satisfy conditions in part 1 of the Theorem 3. It means that the maximal value of these indices over $\mathcal{CP}_n$ is attained in a polyomino chain. By Corollary 2.7 in [11], among all polyomino chains with n squares these indices attain their maximal value in Ln.
On the other hand, the first Zagreb index and the second Zagreb index satisfy conditions in part 2 of Theorem 3. The minimal value of these indices over $\mathcal{CP}_n$ is attained in a polyomino chain. By Corollary 2.7 in [11], among all polyomino chains with n squares these indices attain their minimal value in Ln. ■

	α_1	α_2	α_3	α_4	α_5	α_6	α_7
Randić	-0.03	-0.01	-0.01	-0.03	-0.02	-0.03	-0.01
Sum-connectivity	-0.06	-0.04	-0.04	-0.06	-0.05	-0.06	-0.04
Harmonic	-0.06	-0.02	-0.02	-0.05	-0.03	-0.06	-0.02
Geometric-arithmetic	-0.07	-0.02	-0.02	-0.07	-0.04	-0.07	-0.02
	β_1	β_2	β_3	β_4	β_5	β_6	β_7
First Zagreb	40.0	40.0	40.0	40.0	40.0	40.0	40.0
Second Zagreb	110.0	130.0	100.0	100.0	110.0	100.0	80.0

Table 1: VDB topological indices with L_n as extremal catacondensed polyomino system.

The Theorem 3 cannot be applied on atom-bond-connectivity index and augmented Zagreb index as can be seen from the values showed in the Table 2.

	α_1	α_2	α_3	α_4	α_5	α_6	α_7
Atom-bond-connectivity	0.02	-0.02	0.04	0.02	0.003	0.03	0.07
Augmented Zagreb	179.6	228.2	228.2	176.8	201.2	179.6	228.2
	β_1	β_2	β_3	β_4	β_5	β_6	β_7
Atom-bond-connectivity	-0.07	-0.11	-0.11	-0.07	-0.10	-0.07	-0.11
Augmented Zagreb	52.4	101.1	28.1	22.7	47.0	25.4	-26.0

Table 2: Values of α_i and β_i for atom-bond connectivity and augmented Zagreb indices.

Acknowledgements. The authors are grateful to Fundación para la Promoción de la Investigación y la Tecnología (Banco de la República - 201508) for their generous financial support.

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Received: October 15, 2015; Published: February 19, 2016