The Linear 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 linear chain as an extreme value among all polyomino chains. As a consequence, we deduce that over the polyomino chains, the linear 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 and the second Zagreb index.

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1 Introduction

A topological index is a molecular descriptor which is computed from the molecular graph of a chemical compound. Perhaps the most important one is the Randić index, proposed by Milan Randić [21] for measuring the extent of branching of the carbon-atom skeleton of saturated hydrocarbons. It became
one of the most widely used in applications to physical and chemical properties ([5],[13],[14],[22]). For a survey on the mathematical properties of the Randić index we refer to ([15],[16]).

Let $G$ be a graph with $n$ vertices. We will denote the set of vertices of $G$ by $V(G)$ and the edge set by $E(G)$. The Randić index of $G$ is denoted by $\chi(G)$ and defined as

$$\chi(G) = \sum_{1 \leq i \leq j \leq n-1} m_{ij} \frac{1}{\sqrt{ij}},$$

where $m_{ij}$ denotes the number of $ij$-edges, i.e. edges with end vertices of degree $i$ and $j$. More generally, a vertex-degree-based topological index $TI$ (VDB topological index, for short) is defined from any set of real numbers $\{\varphi_{ij}\}$ as

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

In particular, when $\varphi_{ij} = \frac{1}{\sqrt{ij}}$ we recover the Randić index. Motivated by the success of the Randić index, many other topological indices appeared in the mathematical-chemistry literature which can be obtained from the expression given in (1), for example, the sum-connectivity index is obtained from $\varphi_{ij} = \frac{1}{\sqrt{ij}}$ [28], the harmonic index from $\varphi_{ij} = \frac{2}{i+j}$ [27], the geometric-arithmetic index from $\varphi_{ij} = \frac{2\sqrt{ij}}{i+j}$ [23], the first Zagreb index from $\varphi_{ij} = i + j$ and the second Zagreb index from $\varphi_{ij} = ij$ [8], the atom-bond-connectivity index from $\varphi_{ij} = \sqrt{i+j-2}$ [6] and the augmented Zagreb index from $\varphi_{ij} = \left(\frac{ij}{i+j-2}\right)^3$ [7]. For recent publications on VDB topological indices we refer to ([2],[4],[9],[10],[19],[20]).

Our interest in this paper is to study VDB topological indices over the class of polyomino systems. 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. Applications of the polyomino systems to crystal physics can be found in ([11],[12]). 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. In particular, a linear chain is a polyomino chain with exactly one segment (see Figure 1). We will denote by $L_n$ the linear chain with $n$ squares.

Topological indices over polyomino systems have appeared recently in the literature. ([1], [3], [17], [24], [25], [26]). In our study, we consider VDB
topological indices in its general expression given in (1), and show that under certain conditions imposed to 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. As a consequence, we show that the linear chain has extremal value for many of the well-known vertex-degree-based topological indices.

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

In order to formally introduce the linearizing operations on an angular square of a polyomino chain, we recall the definition of coalescence of two graphs [18]. Suppose that for $i = 1, 2, G_i$ is a graph and $a_i, b_i$ are its two adjacent vertices. Construct the graph $G$ from $G_1$ and $G_2$, by identifying the vertices $a_1$ and $a_2$ and also identifying $b_1$ and $b_2$. Denote by $u^*$ the vertex obtained by coalescing $a_1$ and $a_2$, and by $v^*$ the vertex obtained by coalescing $b_1$ and $b_2$. Then two vertices of $G$ are adjacent if (see Figure 2):

1. they are adjacent in $G_1$ or $G_2$, or
2. if one is $u^*$ and the other one was adjacent to $a_1$ in $G_1$ or to $a_2$ in $G_2$, or
3. if one is $v^*$ and the other was is adjacent to $b_1$ in $G_1$ or $b_2$ in $G_2$, or
4. if one is $u^*$ and the other one is $v^*$.

We compute in our following results the variation of a topological index of the form (1) under linearizing operations. The first operation linearizes at an angular square (shadow square in Figure 3) in which the two adjacent squares are linear.

If $U$ is a polyomino chain and $M$ is a subset of $E(U)$, then we denote by $E(U) \setminus M$ 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 linearizing operation 1 shown in Figure 3, where $X$ is a polyomino chain and $L$ is a linear chain. Then

$$TI(V_1) - TI(U_1) = 6\varphi_{33} - 2\varphi_{23} - 4\varphi_{34}$$
Figure 2: Coalescence of graphs.

Figure 3: Linearizing operation 1.
Proof. Let $M_1$ be the set of edges in bold of $U_1$ and $N_1$ the set of edges in bold in $V_1$ as shown in Figure 3. Then there exist a one-to-one correspondence between the set of edges $E(U_1) \setminus M_1$ and $E(V_1) \setminus N_1$, in such a way that the degrees of the end vertices of every edge in $E(U_1) \setminus M_1$ are equal to those of the correspondent edge in $E(V_1) \setminus N_1$. Since $M_1$ consists of two 23-edges and four 34-edges, and $N_1$ consists of six 33-edges, then

$$TI(V_1) - TI(U_1) = 6\varphi_{33} - (2\varphi_{23} + 4\varphi_{34})$$

$$= 6\varphi_{33} - 2\varphi_{23} - 4\varphi_{34}$$

Operation 2 linearizes at an angular square (shadow square in Figure 4) which is adjacent to a linear and an angular square.

Lemma 2.2 Let $TI$ be a topological index induced by the numbers $\{\varphi_{ij}\}$. Consider the linearizing operation 2 shown in Figure 4, where $X$ is a polyomino chain and $L$ is a linear chain. Then

$$TI(V_2) - TI(U_2) = 3\varphi_{33} - 2\varphi_{24} - \varphi_{44}$$

Proof. Let $M_2$ be the set of edges in bold of $U_2$ and $N_2$ the set of edges in bold in $V_2$ as shown in Figure 4. Then there exist a one-to-one correspondence between the set of edges $E(U_2) \setminus M_2$ and $E(V_2) \setminus N_2$, in such a way that the degrees of the end vertices of every edge in $E(U_2) \setminus M_2$ are equal to those of the correspondent edge in $E(V_2) \setminus N_2$. Since $M_2$ consists of two 34-edges, two 24-edges, one 44-edge and one 23-edge, and $N_2$ consists of three 33-edges, two 34-edges and one 23-edge, then

$$TI(V_2) - TI(U_2) = (\varphi_{23} + 2\varphi_{34} + 3\varphi_{33}) - (2\varphi_{34} + 2\varphi_{24} + \varphi_{44} + \varphi_{23})$$

$$= 3\varphi_{33} - 2\varphi_{24} - \varphi_{44}$$
Now we consider the linearizing operation 3 at an angular square (shadow square in Figure 5) in which one of the adjacent squares is a terminal square and the other is a linear square.

Lemma 2.3 Let $TI$ be a topological index induced by the numbers $\{\varphi_{ij}\}$. Consider the linearizing operation 3 shown in Figure 5, where $X$ is a polyomino chain. Then

$$TI(V_3) - TI(U_3) = 5\varphi_{33} - 3\varphi_{34} - \varphi_{24} - \varphi_{23}$$

Proof. Let $M_3$ be the set of edges in bold of $U_3$ and $N_3$ the set of edges in bold in $V_3$ as shown in Figure 5. Then there exist a one-to-one correspondence between the set of edges $E(U_3) \setminus M_3$ and $E(V_3) \setminus N_3$, in such a way that the degrees of the end vertices of every edge in $E(U_3) \setminus M_3$ are equal to those of the correspondent edge in $E(V_3) \setminus N_3$. Since $M_3$ consists of three 34-edges, two 23-edges and one 24-edge, and $N_3$ consists of five 33-edges and one 23-edge, then

$$TI(V_3) - TI(U_3) = (5\varphi_{33} + \varphi_{23}) - (3\varphi_{34} + \varphi_{24} + 2\varphi_{23}) = 5\varphi_{33} - 3\varphi_{34} - \varphi_{24} - \varphi_{23}$$

Finally, operation 4 linearizes at an angular square (shadow square in Figure 6) in which one adjacent square is a terminal square and the other is an angular square.

Lemma 2.4 Let $TI$ be a topological index induced by the numbers $\{\varphi_{ij}\}$. Consider the linearization operation 4 shown in Figure 6, where $X$ is a polyomino chain. Then

$$TI(V_4) - TI(U_4) = \varphi_{23} + 2\varphi_{33} + \varphi_{34} - 3\varphi_{24} - \varphi_{44}$$

Proof. Let $M_4$ be the set of edges in bold of $U_4$ and $N_4$ the set of edges in bold in $V_4$ as shown in Figure 6. Then there exist a one-to-one correspondence
Figure 6: Linearizing operation 4.

between the set of edges $E(U_4) \setminus M_4$ and $E(V_4) \setminus N_4$, in such a way that the degrees of the end vertices of every edge in $E(U_4) \setminus M_4$ are equal to those of the correspondent edge in $E(V_4) \setminus N_4$. Since $M_4$ consists of three 24-edges, one 34-edges, one 44-edge and one 23-edge, and $N_4$ consists of two 23-edges, two 33-edges and two 34-edges, then

$$TI(V_4) - TI(U_4) = (2\varphi_{23} + 2\varphi_{33} + 2\varphi_{34}) - (3\varphi_{24} + \varphi_{34} + \varphi_{23} + \varphi_{44})$$

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

Based on the four operations given above we next show that the linear polyomino chain has extremal $TI$ value among all polyomino chains with a fixed number of squares. But first we illustrate this with an example.

**Example 2.5** In Figure 7 we show how to construct a sequence of polyomino chains using operations 1-4 given above to reach the linear chain. In each step we apply the operation over the first angular square that appears in the chain, represented with a shadowed square. The number in the rectangle is the number of squares in the linear chain.

Now we can show the main result, the proof is following the idea of Example 2.5.

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

1. If

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

then $L_n$ has maximal $TI$-value among all polyomino chains of $n$ squares.
2. If
\[
\begin{align*}
6\varphi_{33} - 2\varphi_{23} - 4\varphi_{34} &\leq 0 \\
3\varphi_{33} - 2\varphi_{24} - \varphi_{44} &\leq 0 \\
5\varphi_{33} - 3\varphi_{34} - \varphi_{24} - \varphi_{23} &\leq 0 \\
\varphi_{23} + 2\varphi_{33} + \varphi_{34} - 3\varphi_{24} - \varphi_{44} &\leq 0
\end{align*}
\]
then $L_n$ 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 $L_n$. We use induction on the number of segments $s$ of the polyomino chain $P$. If $s = 1$ then $P = L_n$ and we are done. Assume that the result holds for $s \geq 1$ and let $P$ be a polyomino chain with $s + 1$ segments. Choose the first angular square that appears in $P$. Then $P$ is of the form $U_i$ for some $i = 1, 2, 3$ or 4 in Figures 3-6. Then by our hypothesis $TI(V_i) - TI(U_i) \geq 0$ and clearly $V_i$ has $s$ segments. Then by our induction hypothesis $TI(V_i) \leq TI(L_n)$ and so
\[
TI(P) = TI(U_i) \leq TI(V_i) \leq TI(L_n)
\]

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 maximal value in $L_n$. The first Zagreb index and the second Zagreb index attain the minimal value in $L_n$.

**Proof.** The values of
\[
\begin{align*}
6\varphi_{33} - 2\varphi_{23} - 4\varphi_{34} &\quad (2) \\
3\varphi_{33} - 2\varphi_{24} - \varphi_{44} &\quad (3) \\
5\varphi_{33} - 3\varphi_{34} - \varphi_{24} - \varphi_{23} &\quad (4) \\
\varphi_{23} + 2\varphi_{33} + \varphi_{34} - 3\varphi_{24} - \varphi_{44} &\quad (5)
\end{align*}
\]
are calculated in the following table:

<table>
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<th>(3)</th>
<th>(4)</th>
<th>(5)</th>
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<tr>
<td>Randić</td>
<td>.028803</td>
<td>.042893</td>
<td>.038840</td>
<td>.052930</td>
</tr>
<tr>
<td>Sum-connectivity</td>
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<td>.054695</td>
<td>.051886</td>
<td>.063376</td>
</tr>
<tr>
<td>Harmonic</td>
<td>.057143</td>
<td>.083333</td>
<td>.07619</td>
<td>.10238</td>
</tr>
<tr>
<td>Geometric-arithmetic</td>
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<td>.11438</td>
<td>.10817</td>
<td>.14111</td>
</tr>
<tr>
<td>First Zagreb</td>
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<td>-2</td>
<td>-2</td>
<td>-2</td>
</tr>
<tr>
<td>Second Zagreb</td>
<td>-6</td>
<td>-5</td>
<td>-5</td>
<td>-4</td>
</tr>
</tbody>
</table>
As we can see, the Randić index, the sum-connectivity index, the harmonic index and the geometric-arithmetic index satisfy the conditions in part 1 of Theorem 2.6, while the first Zagreb index and the second Zagreb index satisfy conditions in part 2 of Theorem 2.6. We note that we cannot apply Theorem 2.6 on the atom-bond-connectivity index and the augmented Zagreb index since

<table>
<thead>
<tr>
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<th>(2)</th>
<th>(3)</th>
<th>(4)</th>
<th>(5)</th>
</tr>
</thead>
<tbody>
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<td>Atom-bond-connectivity</td>
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<td>−0.026586</td>
<td>−0.017372</td>
<td>−0.047755</td>
</tr>
<tr>
<td>Augmented Zagreb</td>
<td>−2.9523</td>
<td>−0.79109</td>
<td>−0.51888</td>
<td>1.6423</td>
</tr>
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In fact, the unique polyomino chain with three squares different from the linear chain has atom-bond-connectivity index smaller than the linear chain. Similarly occurs with the augmented Zagreb index.

References


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