On Sum-Connectivity Index of Polyomino Chains

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Abstract

If $G$ is a (molecular) graph with $n$ vertices, and $d_i$ is the degree of its $i$-th vertex, then the sum-connectivity index of $G$ is the sum of the weights $(d_u + d_v)^{-\frac{1}{2}}$ of all edges $uv$ of $G$. A polyomino system is a finite 2-connected plane graph such that each interior face (or say a cell) is surrounded by a regular square of length one. Formulas for calculating the sum-connectivity index of polyomino chains are provided.

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1 Introduction

The structure of a molecule could be represented in a variety of ways. The information on the chemical constitution of molecule is conventionally represented by a molecular graph. And graph theory was successfully provided the chemist with a variety of very useful tools, namely, topological indices. One of the oldest and most thoroughly examined molecular graph-based structural descriptor of organic molecule is the Wiener index or Wiener number [1].

In 1975, Randić introduced a molecular structure-descriptor in his study of alkanes[2] which he called the branching index, and is now called the the Randić index, is a graph-based molecular structure descriptor that is most frequently applied in quantitative structure-property and structure-activity studies[2-6]. It is defined as the sum over all edges of the (molecular) graph of the terms $(d_ud_v)^{-\frac{1}{2}}$, where $u$ and $v$ are the vertices of the edge $uv \in E(G)$, and $d_u$ (or $d_v$) is the degree of the vertex $u$ (or $v$), i.e.,

$$R(G) = \sum_{uv \in E(G)} (d_ud_v)^{-\frac{1}{2}} \quad (1)$$
The Randić index has been closely correlated with many chemical properties [3-6].

The sum-connectivity index of the graph $G$, denoted by $\chi(G)$, is defined as[7]:

$$\chi(G) = \sum_{uv \in E(G)} (d_u + d_v)^{-\frac{1}{2}}$$ (2)

Let $ij$ denotes the edge with degree $i$, $j$, resp. The sum-connectivity index can be rewritten as

$$\chi(G) = \sum_{i \sim j} \frac{1}{\sqrt{i + j}}$$

Sum-connectivity index belongs to a family of Randić-like indices, is a new variant of the famous Randić connectivity index usable in quantitative structure-property relationship and quantitative structure-activity relationship studies, the uses of the sum-connectivity index in modeling a number of molecular properties is presented in the monograph entitled Novel Molecular Structure Descriptors - Theory and Applications I, edited by Gutman and Furtula[10].

For convenience, we might sometimes call $R(G)$ the product-connectivity index of $G$. These two molecular descriptors are highly intercorrelated quantities[8]. In [7], the authors provided several basic properties for sum-connectivity index, especially lower and upper bounds in terms of sum-connectivity index, determined the unique tree with given numbers of vertices and pendant vertices with the minimum value of the sum-connectivity index, and trees with the minimum, second minimum and third minimum, and with the maximum, second maximum and third maximum values of the sum-connectivity index, and discussed properties of the sum-connectivity index for a class of trees representing acyclic hydrocarbons. In [9], some properties of the sum-connectivity index for trees and unicyclic graphs with given matching number were obtained.

In the paper, we will give formulas for calculating the sum-connectivity index of polyomino chains.

## 2 Preliminary Notes

A polyomino system is a finite 2-connected plane graph such that each interior face (or say a cell) is surrounded by a regular square of length one. In other words, it is an edge-connected union of cells in the planar square lattice. A polyomino chain is a polyomino system, in which the joining of the centers of its adjacent regular forms a path $c_1c_2\cdots c_n$, where $c_i$ is the center of the $i$-th square. Let $B_n$ be the set of polyomino chains with $n$ squares, the number of edges in $B_n$ is $3n + 1$. $B_n \in B_n$. If the subgraph of $B_n$ induced by the vertices with degree 3 is a graph with exactly $n - 2$ squares, then $B_n$ is called a linear
chain and denoted by $L_n$. If the subgraph of $B_n$ induced by the vertices with
degree bigger than two is a path with $n - 1$ edges, then $B_n$ is called a zig-zag
chain and denoted by $Z_n$.

A kink of a polyomino chain is the branched or angularly connected squares.
A segment of a polyomino chain is a maximal linear chain in the polyomino
chains, including the kinks and/or terminal squares at its end. The number
of squares in a segment $S$ is called its length and is denoted by $l(S)$. For
any segment $S$ of a polyomino chain with $n \geq 2$ squares, $2 \leq l(S) \leq n$.
Particularly, for a linear chain $L_n$ with $n$ squares, we have $s = 1$ and $l_1 = n$.
For a zig-zag chain $Z_n$ with $n$ squares, we have $s = n - 1$ and $l_1 = 2$.

A polyomino chain consists of a sequence of segments $S_1, S_2, \ldots, S_s$, $s \geq 1$,
with lengths $l(S_i) = l_i$, $i = 1, 2, \ldots, s$, where $l_1 + l_2 + \cdots + l_s = n + s - 1$(where
$n$ denote the number of squares of a polyomino chain) since two neighboring
segments have always one square in common.

### 3 The sum-connectivity index of polyomino
chains

In following, we shall calculating the sum-connectivity index of polyomino
chains.

**Theorem 3.1** Let $L_n, Z_n$ be the polyomino chains depicted in Figure 1. Then

\[
\chi(L_n) = \begin{cases} 
2, & n = 1; \\
1 + \frac{4\sqrt{7}}{3} + \frac{\sqrt{7}}{6}(3n - 5), & n \geq 2.
\end{cases}
\]

\[
\chi(Z_n) = \begin{cases} 
2, & n = 1; \\
1 + \frac{4\sqrt{7}}{3} + \frac{\sqrt{7}}{6}, & n = 2; \\
\left(\frac{\sqrt{2}}{4} + \frac{\sqrt{6}}{3}\right)n + 1 + \frac{4\sqrt{7}}{5} + \frac{2\sqrt{7}}{7} - \frac{2\sqrt{6}}{3} - \frac{3\sqrt{7}}{4}, & n \geq 3.
\end{cases}
\]

**Proof.** When $n = 1, 2$, it is suffice to see the results, in our following
discussion, we assume that $n \geq 3$.

The total number of edges in $L_n$ and $Z_n$ is $3n + 1$. Let $n_{ij}$ be the number
of edges with degree $i, j$. Thus,

(i) For the polyomino chain $L_n$, $n_{22} = 2$, $n_{23} = 4$ and $n_{33} = 3n + 1 - (2 + 4) = 3n - 5$. By the definition of Randić index, we have

\[
\chi(L_n) = \sum_{1 \leq i, j \leq n-1} \frac{1}{\sqrt{i+j}} = \frac{2}{\sqrt{2+2}} + \frac{4}{\sqrt{2+3}} + \frac{3n-5}{\sqrt{3+3}} = 1 + \frac{4\sqrt{7}}{5} + \frac{\sqrt{7}}{6}(3n - 5)
\]

(ii) By the same way, we have

\[
\chi(Z_n) = \left(\frac{\sqrt{2}}{4} + \frac{\sqrt{6}}{3}\right)n + 1 + \frac{4\sqrt{7}}{5} + \frac{2\sqrt{7}}{7} - \frac{2\sqrt{6}}{3} - \frac{3\sqrt{7}}{4}
\]
Theorem 3.2 Let $B^1_n(n \geq 3)$ be a polyomino chain with $n$ squares and consisting of $s$ segments $S_1, S_2$ with lengths $l_1 = 2, l_2 = n - 1$. Then

$$
\chi(B^1_n) = \begin{cases} 
1 + \frac{4\sqrt{5}}{5} + \frac{\sqrt{6}}{3} + \frac{2\sqrt{7}}{7}, & n = 3; \\
\frac{\sqrt{6}}{2} n + 1 + \sqrt{5} + \frac{3\sqrt{7}}{7} - \frac{3\sqrt{6}}{2}, & n \geq 4.
\end{cases}
$$

Proof. For $n = 3$, it is trivial, we omit it here. When $n \geq 4$, it is suffice to see that, $n_{22} = 2, n_{23} = 5, n_{24} = 1, n_{34} = 3, n_{33} = 3n + 1 - 2 - 5 - 1 - 3 = 3n - 10$. Thus

$$
\chi(B^2_n) = \frac{2}{\sqrt{2+2}} + \frac{5}{\sqrt{2+3}} + \frac{1}{\sqrt{2+4}} + \frac{3}{\sqrt{3+4}} + \frac{3n-10}{\sqrt{4+4}}
$$

In our following discussion, we assume that $2 \leq l(i) \leq n - 1$ with $1 \leq i \leq s$.

Theorem 3.3 Let $B^2_n(n \geq 4)$ be a polyomino chain with $n$ squares and consisting of $s$ segments $S_1, S_2, \cdots, S_s$ ($s \geq 3$) with lengths $l_1 = l_s = 2, l_2, \cdots, l_{s-1} \geq 3$. Then

$$
\chi(B^2_n) = \begin{cases} 
\frac{5}{4} + \frac{2\sqrt{11}}{3} + \frac{\sqrt{6}}{3} + \sqrt{2}, & n = 4; \\
\frac{3\sqrt{6}}{4} n + (\frac{2\sqrt{5}}{6} + \frac{4\sqrt{7}}{7} - \frac{3\sqrt{6}}{2}) s + 1 + \frac{\sqrt{6}}{3} + \frac{3\sqrt{7}}{4} - \frac{6\sqrt{5}}{7}, & n \geq 5.
\end{cases}
$$

Proof. When $n = 4$, it is trivial. We assume $n \geq 5$. In $B^2_n$, we know $n_{22} = 2, n_{23} = 2s, n_{24} = 2, n_{34} = 4s - 6, n_{33} = 3n + 1 - 2 - 2s - 2 - (4s - 6) = 3n - 6s + 3$. Thus

$$
\chi(B^2_n) = \frac{2}{\sqrt{2+2}} + \frac{2s}{\sqrt{2+3}} + \frac{2}{\sqrt{2+4}} + \frac{4s-6}{\sqrt{3+4}} + \frac{3n-6s+3}{\sqrt{4+4}}
$$

Similarly, we have

Theorem 3.4 Let $B^3_n$ be a polyomino chain with $n$ squares and consisting of $s$ segments $S_1, S_2, \cdots, S_s$ ($s \geq 3$) with lengths $l_1 = 2, l_2, \cdots, l_{s-1}, l_s \geq 3$ or $l_s = 2, l_1, l_2, \cdots, l_{s-1} \geq 3$. Then

$$
R(B^3_n) = \frac{\sqrt{6}}{2} n + (\frac{2\sqrt{5}}{5} + \frac{4\sqrt{7}}{7} - \sqrt{6}) s + 1 + \frac{\sqrt{5}}{5} + \frac{2\sqrt{6}}{3} - \frac{5\sqrt{7}}{7}
$$

Theorem 3.5 Let $B^4_n$ be a polyomino chain with $n$ squares and consisting of $s$ segments $S_1, S_2, \cdots, S_s$ ($s \geq 3$) with lengths $l_i \geq 3 (i = 1, 2, \cdots, s)$. Then

$$
R(B^4_n) = \frac{\sqrt{6}}{2} n + (\frac{2\sqrt{5}}{5} + \frac{4\sqrt{7}}{7} - \sqrt{6}) s + 1 + \frac{2\sqrt{5}}{5} + \frac{\sqrt{6}}{6} - \frac{4\sqrt{7}}{7}
$$

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References


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