Int. J. Nonlinear Anal. Appl. 17 (2026) 2, 111–116
ISSN: 2008-6822 (electronic)
http://dx.doi.org/10.22075/ijnaa.2023.29433.4164

A classification of total irregularity of polyomino chains based on segments by using non-decreasing real function

Zahra Yarahmadi

Department of Mathematics, Khorramabad Branch, Islamic Azad University, Khorramabad, Iran

(Communicated by Mohammad Bagher Ghaemi)

Abstract

The total irregularity is a type of graph invariant and for a given simple graph G is calculated by the formula, $irr_t(G) = \frac{1}{2}\sum_{\{u,v\}\subseteq V(G)} \mid deg_G u - deg_G v \mid$, in which $deg_G v$ is the degree of the vertex v of G. This paper aims to offer a classification of polyomino chains based on segments in terms of total irregularity. We can find a sequence for all polyomino chains concerning this graph invariant by defining a non-decreasing function.

Keywords: Total irregularity, polyomino chain
2020 MSC: 05C07, 05C35

1 Introduction and Preliminaries

Let G be a simple and undirected graph, with vertex set $V(G)$ and edge set $E(G)$. If a and b are two adjacent vertices, then the edge connecting them is denoted by $e = ab$. The degree of a vertex a is denoted by $deg_G a$. When the graph under discussion is obvious in context, the subscript G will be omitted. The degree-based graph invariants are parameters defined by degrees of vertices. Gutman and Trinajestic introduced the first graph parameters more than thirty years ago, [8]. The Zagreb indices were originally defined as follows:

$$M_1(G) = \sum_{u\in V(G)} deg_G^2 u,$$

$$M_2(G) = \sum_{e=uv\in E(G)} deg_G u \, deg_G v.$$

Here, $M_1(G)$ and $M_2(G)$ denote the first and the second Zagreb index, respectively. Alternatively the first Zagreb index can be expressed as

$$M_1(G) = \sum_{e=uv\in E(G)} [deg_G u + deg_G v].$$

We refer the reader to [10] for the proof of this equation. These indices have a long history; interested readers can look up additional information on Zagreb indices in [7, 10, 17, 16, 18]. The number $\mid deg_G a - deg_G b \mid$ is an important

Email address: zahra.yarahmadi@iau.ac.ir, z.yarahmadi@gmail.com (Zahra Yarahmadi)

Received: December 2022 *Accepted:* January 2023

parameter associated with the edge e. This number is defined as the imbalance of the edge $e = ab$. In [4], Albertson defined the irregularity of G as $irr(G) = \frac{1}{2}\sum_{e=uv\in E(G)} \mid deg_G u - deg_G v \mid$. The total irregularity of a graph G was introduced by Abdo et al. [1] as $irr_t(G) = \frac{1}{2}\sum_{\{u,v\}\subseteq V(G)} \mid deg_G u - deg_G v \mid$. They obtained all graphs G such that $irr_t(G)$ are the maximum possible value for them, and proved that among all trees of the same order, the star has the maximal total irregularity.

Theorem 1.1. [1] For a simple undirected graph G with n vertices, it holds that:

$$irr_t(G) \leq \begin{cases} \frac{1}{12}(2n^3 - 3n^2 - 2n + 3) & n \, is \, odd \\ \frac{1}{12}(2n^3 - 3n^2 - 2n) & n \, is \, even \end{cases} .$$

It is usual to assume that a graph invariant f is a measure of irregularity, when $f(G) = 0$ if and only if G is regular. Since the irregularity and total irregularity are zero if and only if G is regular, they are measures of irregularity for graphs. Furthermore, $irr_t(G)$ is an upper bound of $irr(G)$. Dimitrov [5], compared these two important measures of irregularity and proved that $irr_t(G) \leq n^2\frac{irr(G)}{4}$, when G is an n-vertex connected graph. Moreover, for an arbitrary n-vertex tree G, we have $irr_t(G) \leq (n-2)irr(G)$. For more information about results on total irregularity of graphs, see [3, 6, 14, 19]. A plane graph is a graph can be embedded on a sphere in such a way that edges intersect each other only in vertices of the graph. A connected graph G is called 2−connected, if for each vertex a, $G - a$ is connected. A finite 2−connected plane graph such that each interior face is surrounded by a regular square of length one is said to be a polyomino system. Polyominoes have a long and rich history, we convey for the origin polyominoes, Klarner [9]. A polyomino chain is a polyomino system, in which the joining of the centers of its adjacent regular forms a path $c_1c_2...c_n$, where c_i is the center of the i−th square. Let $\mathbf{B_n}$ be the set of polyomino chains with n squares. For $B_n \in \mathbf{B_n}$, it is easy to see that $|V(B_n)| = 2n + 2$ and $|E(B_n)| = 3n + 1$.

The following introduces some key notions concerning polyomino chains that will be useful later. A polyomino chain square can have one or two surrounding squares. A square is called terminal if it has only one nearby square, and kink if it has two neighboring squares and a vertex of degree 2. In Figure 1, the kinks are denoted by the letter K. The linear chain is a kink-free polyomino chain, see Figure 2.

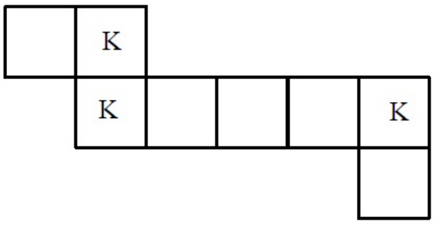

Figure 1: The kinks.

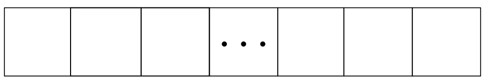

Figure 2: A linear chain.

A maximal linear chain in a polyomino chain is called a segment, if it includes the kinks and/or terminal squares at its end. The length of a segment S, $l(S)$, is the number of squares in S. Note that for each segment S of a polyomino chain with $n \geq 2$ squares, $2 \leq l(S) \leq n$. A polyomino chain with n squares consists of a sequence of segments $S_1, S_2, ..., S_r$, $1 \leq r \leq n$, with lengths $l(S_i) = l_i$, $1 \leq i \leq r$, where $l_1 + l_2 + ... + l_r = n + r - 1$. In Figure 3, the squares on each segments of a polyomino chain is shown by directional lines.

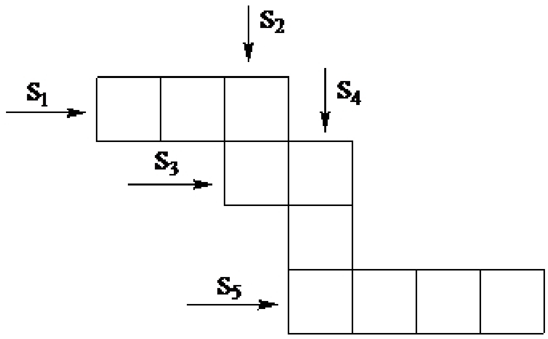

Figure 3: Segments of a polyomino chain.

A zigzag chain Z_n with n squares is a polyomino with $n-2$ kinks and in another word, a polyomino chain is a zigzag chain if and only if the length of each segment is 2 , see Figure 4.

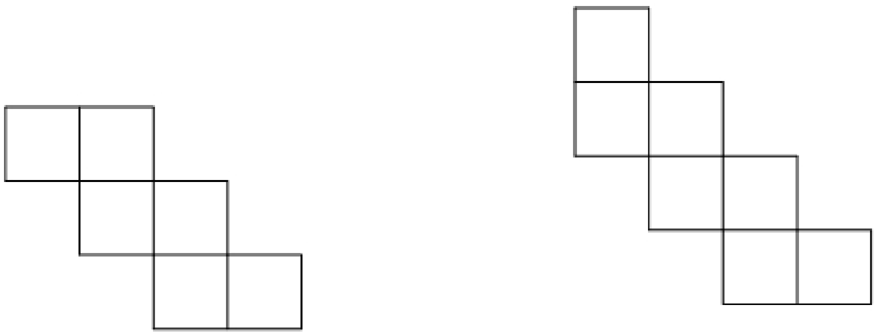

Figure 4: The zigzag chains Z_6 and Z_7.

Xu and Chen were studied the PI index of polyomino chains, [11]. After that Chen et.al. continue this program to other topological indices, see [12, 13]. Present author in [15] continue this line of research by calculation the first and second Zagreb indices of polyomino chains and then determine extremal polyomino chains with respect to Zagreb indices. In [2], authors present split formula for total irregularity of polyomino chain. In this paper, we are interested in finding relation between the number of segments and total irregularity of polyomino chains. We classify polyomino chains based on segments by new approach and using non-decreasing real function.

2 Main results

The purpose of this section is to categorize polyomino chains according to their total irregularity based on segments. We begin by calculating the overall irregularity of polyomino chains, We have obtained it in a different method from the proof presented in [2]. Following that, we'll look at total irregularity's behavior in relation to the number of segments in each polyomino chain. The total irregularity of G is defined as:

$$irr_t(G) = \frac{1}{2} \sum_{\{u,v\} \subseteq V(G)} \mid deg_G u - deg_G v \mid,$$

where $deg_G v$ is the degree of the vertex v of G. It is easy to know that, for any $B_n \in \mathbf{B_n}$, $\{deg_{B_n} u \mid u \in V(B_n)\} = \{2, 3, 4\}$. We will denote by n_2, n_3 and n_4, the number of vertices of degree 2, 3 and 4, respectively. It is obvious that, $n_2 \geq 4$, $n_3 \geq 2$ and $|V(B_n)| = n_2 + n_3 + n_4$. For attaining the results of this paper, firstly we consider the following useful lemma.

Lemma 2.1. For every $B_n \in \mathbf{B_n}$, the following formula is hold:

$$irr_t(B_n) = \frac{1}{2}\big(n_2n_3 + 2n_2n_4 + n_3n_4\big).$$

Proof . We begin by defining the following sets:

$$\begin{aligned}
A_1 &= \big\{\{u,v\} \subseteq V(B_n) | deg_{B_n}u = deg_{B_n}v\big\},\\
A_2 &= \big\{\{u,v\} \subseteq V(B_n) | \{deg_{B_n}u, deg_{B_n}v\} = \{2,3\}\big\},\\
A_3 &= \big\{\{u,v\} \subseteq V(B_n) | \{deg_{B_n}u, deg_{B_n}v\} = \{2,4\}\big\},\\
A_4 &= \big\{\{u,v\} \subseteq V(B_n) | \{deg_{B_n}u, deg_{B_n}v\} = \{3,4\}\big\}.
\end{aligned}$$

Of course clearly, $\sum_{A_1} \mid deg_{B_n}u - deg_{B_n}v \mid= 0$, $\sum_{A_2} \mid deg_{B_n}u - deg_{B_n}v \mid= n_2n_3$, $\sum_{A_3} \mid deg_{B_n}u - deg_{B_n}v \mid= 2n_2n_4$ and finally, in the same manner, we can see $\sum_{A_4} \mid deg_{B_n}u - deg_{B_n}v \mid= n_3n_4$.

Then, by definition of total irregularity of B_n and according above arguments, we have:

$$\begin{aligned}
irr_t(B_n) &= \frac{1}{2} \sum_{\{u,v\}\subseteq V(B_n)} |deg_{B_n}u - deg_{B_n}v|\\
&= \frac{1}{2} \sum_{i=1}^{4} \sum_{A_i} |deg_{B_n}u - deg_{B_n}v|\\
&= \frac{1}{2}\big(n_2n_3 + 2n_2n_4 + n_3n_4\big).
\end{aligned}$$

□

Now we can apply the above conclusions to special case of polyomino chains and calculate the total irregularity of linear and zigzag chains. It is easy to see that, $irr_t(L_n) = 4n - 4$ and $irr_t(Z_n) = n^2 + 2n - 4$. The continuing of computing total irregularity of polyomino chains is established by our theorem. In the following theorem, we obtain total irregularity of polyomino chains according the number of segments and squares.

Theorem 2.2. Let B_n be a polyomino chain with n squares and r segments. Then,

$$irr_t\big(B_n\big) = -r^2 + 2rn + 2n - 3.$$

Proof . Let us first prove the following statement $P(n)$ by induction on natural number n.

$P(n)$:" For each polyomino chain with n squares and r segments, $n_2 = r + 3$, $n_3 = 2n - 2r$ and $n_4 = r - 1$."

obviously the statement $P(n)$ holds for $n = 1$. To prove the inductive step, one assumes the induction hypothesis for n and then uses this assumption to prove that the statement holds for $n + 1$. Assume that B_{n+1} be a polyomino chain with $n + 1$ squares and k segments, the statement P_{n+1} is as follows for B_{n+1}

P_{n+1} : "For polyomino chain B_{n+1} with $n+1$ squares and k segments, $n_2 = k+3$, $n_3 = 2n-2k+2$ and $n_4 = k-1$."

Remove one of a terminal square of B_{n+1}. By this removing, we obtain a polyomino chain with n squares, call it B_n. There are two cases for B_n:

Case 1: If removing terminal square be in the segment S of length rather than 2, ($l(S) > 2$) in B_{n+1}, then B_n has k segments, see Figure 5. By hypothesis induction we have $n'_2 = k + 3$, $n'_3 = 2n - 2k$ and $n'_4 = k - 1$, in which n'_2, n'_3 and n'_4 are the number of vertices of degree 2, 3 and 4, respectively. Now by adding removed square and creating B_{n+1} again, one can see that the number of vertices of degree 2 and 4 are not changed and just the number of vertices of degree 3 are increased. Because $v_1, v_2 \in V(B_{n+1})$ as vertices of degree 2 are added to B_n. Since $deg_{B_n}v_3 = deg_{B_n}v_4 = 2$ and $deg_{B_{n+1}}v_3 = deg_{B_{n+1}}v_4 = 3$, then v_3 and v_4 aren't vertices of degree 2 in B_{n+1}. It is easy to check that $n_2 = n'_2 = k + 3$, $n_3 = n'_3 + 2 = 2n - 2k + 2$ and $n_4 = n'_4 = k - 1$. Hence, the statement $P(n + 1)$ is hold for B_{n+1}.

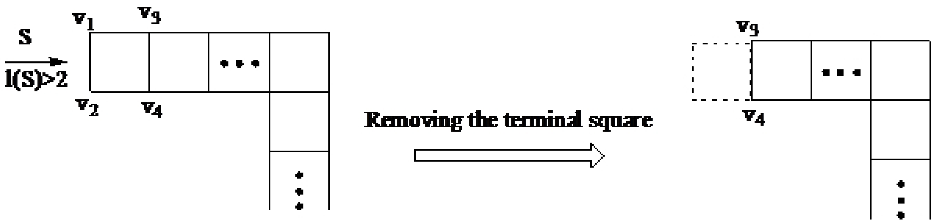

Figure 5: Removing terminal square in Case 1.

Case 2: If removing square be in a segment S of length 2 in B_{n+1}, then B_n has $k-1$ segments, see Figure 6. By hypothesis induction, the number of vertices of degree 2, 3 and 4 are as $n'_2 = k+2$, $n'_3 = 2n-2k+2$ and $n'_4 = k-2$, respectively. Add removed square to create B_{n+1} again. So one added to the vertices of degree 2 and 4 , but the number of the vertices of degree 3 is not changed. Because $v_1, v_2 \in V(B_{n+1})$ as vertices of degree 2 are are added, also $deg_{B_n} v_3 = 2$ and $deg_{B_{n+1}} v_3 = 3$, moreover, $deg_{B_{n+1}} v_3 = 3$ and $deg_{B_{n+1}} v_4 = 4$. It is a simple matter to check that $n_2 = n'_2 + 1 = k+3$, $n_3 = n'_3 = 2n-2k+2$ and $n_4 = n'_4 + 1 = k-1$. In this case as well the statement $P(n+1)$ is hold for B_{n+1}.

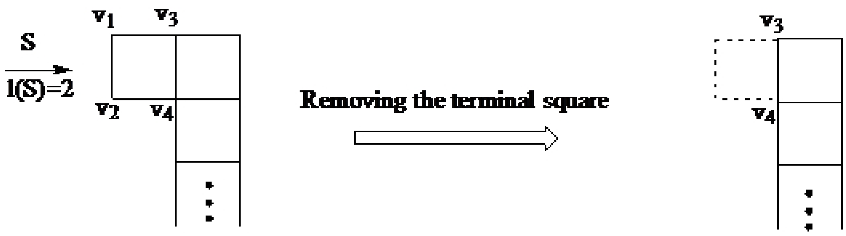

Figure 6: Removing terminal square in Case 2.

By above argument about statement $P(n)$ and Lemma 2.1, we have

$$\begin{aligned} irr_t(B_n) &= \frac{1}{2}\big(n_2 n_3 + 2n_2 n_4 + n_3 n_4\big) \\ &= \frac{1}{2}\big((r+3)(2n-2r) + 2(r+3)(r-1) + (2n-2r)(r-1)\big) \\ &= -r^2 + 2rn + 2n - 3. \end{aligned}$$

□

We denote a polyomino chain with n squares and r segments by B_n^r, clearly $1 \le r \le n-1$.It is necessary to note that B_n^1 and B_n^{n-1} be linear and zigzag chain with n squares.

Corollary 2.3. The following are hold:

$$\begin{aligned} irr_t(B_n^1) &= 4n-4 \\ irr_t(B_n^2) &= 6n-7 \\ &\vdots \\ irr_t(B_n^{n-1}) &= n^2+2n-4. \end{aligned}$$

In the following theorem, we define a non-decreasing real function and use it to achieve our desired classification.

Theorem 2.4. Let B_n^r and B_n^{r-1} be polyomino chain with n squares and r and $r-1$ segments, respectively. Then

$$irr_t(B_n^{r-1}) < irr_t(B_n^r).$$

Proof . We define the function $f : \Re \longrightarrow \Re$, by $f(x) = -x^2+2rn+2n-3$. One can see that $f'(x) = -2r+2n > 0$ on $[1, n-1]$, so f is strictly non-decreasingre function. Thus, for every $x, x-1 \in [1, n-1]$, we get $f(x) < f(x-1)$. By using Theorem 2.3, $irr_t\big(B_n^{r-1}\big) = f(r-1)$ and $irr_t\big(B_n^r\big) = f(r)$ for $r, r-1 \in [1, n-1] \cap \mathbf{N}$. Therefore $irr_t\big(B_n^{r-1}\big) < irr_t\big(B_n^r\big)$ and this completes the proof. □

Corollary 2.5. (i) Let B_n^r be a polyomino chain with n squares and r segments, for $1 \leq r \leq n-1$.The following inequalities are hold:

$$irr_t\big(B_n^1\big) < irr_t\big(B_n^2\big) < \cdots < irr_t\big(B_n^{n-1}\big).$$

(ii) For any $B_n \in \mathbf{B_n}$, $irr_t(L_n) \leq irr_t(B_n) \leq irr_t(Z_n)$, with right (left) equality if and only if $B_n \cong Z_n$ ($B_n \cong L_n$).

References

[1] H. Abdo, S. Brandt, and D. Dimitrov, *The total irregularity of a graph*, Discrete Math. Theor. Comput. Sci. **16** (2014), no. 1, 201–206.

[2] A. Ali, A.A. Bhatti, and Z. Raza, *Some vertex-degree-based topological indices of polyomino chains*, J. Comput. Theor. Nanosci. **12** (2015), no. 9, 2101–2107.

[3] A.R. Ashrafi and A. Ghalavand, *Note on non-regular graphs with minimal total irregularity*, Appl. Math. Comput. **369** (2020), 124891.

[4] M. Albertson, *The irregularity of a graph*, Ars Comb. **46** (1997), 219–225.

[5] D. Dimitrov and R. Škrekovski, *Comparing the irregularity and the total irregularity of graphs*, Ars Math. Contemp. **9** (2015), 45–50.

[6] A. Ghalavand and A.R. Ashrafi, *Ordering of c-cyclic graphs with respect to total irregularity*, J. Appl. Math. Comput. **63** (2020), 707–715.

[7] I. Gutman and K.C. Das, *The first Zagreb index 30 years after*, MATCH Commun. Math. Comput. Chem. **50** (2004), 83–92.

[8] I. Gutman and N. Trinajstic, *Graph theory and molecular orbitals, Total $\pi-$electron energy of alternant hydrocarbons*, Chem. Phys. Lett. **17** (1972), 535–538.

[9] D.A. Klarner, *Polyominoes*, J. E. Goodman and J. O'Rourke (Eds.), Handbook of Discrete and Computational Geometry, CRC Press LLC, Boca Raton, Florida, 1997

[10] S. Nikolic, G. Kovacevic, A. Milicevic, and N. Trinajstic, *The Zagreb indices 30 years after*, Croat. Chem. Acta **76** (2003), 113–124.

[11] L. Xu and S. Chen, *The PI index of polyomino chains*, Appl. Math. Lett. **21** (2008), 1101–1104.

[12] J. Yang, F. Xia and S. Chen, *On the Randić index of polyomino chains*, Appl. Math. Sci. **5** (2011), no. 5, 255–260.

[13] J. Yang, F. Xia, and S. Chen, *On sum-connectivity index of polyomino chains*, Appl. Math. Sci. **5** (2011), no. 6, 267–271.

[14] Z. Yarahmadi, *Finding extremal total irregularity of polyomino chain by transformation method*, J. New Res. Math. **7** (2021), 141–149.

[15] Z. Yarahmadi, A.R. Ashrafi, and S. Moradi, *Extremal polyomino chains with respect to Zagreb indices*, Appl. Math. Lett. **25** (2012), 166–171.

[16] B. Zhou, *Zagreb indices*, MATCH Commun. Math. Comput. Chem. **52** (2004), 113–118.

[17] B. Zhou and I. Gutman, *Relations between Wiener, hyper-Wiener and Zagreb indices*, Chem. Phys. Lett. **394** (2004), 93–95.

[18] B. Zhou and I. Gutman, *Further properties of Zagreb indices*, MATCH Commun. Math. Comput. Chem. **54** (2005), 233–239.

[19] Y. Zhu, L. You, and J. Yang, *The minimal total irregularity of some classes of graphs*, Filomat **30** (2016), 1203–1211.