The expected values of Wiener indices in random polygonal chains

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Abstract

The Wiener index of a graph is a distance-based topological index defined as the sum of distances between all pairs of vertices. In this paper, two explicit expressions for the expected value of the Wiener indices of two types of random polygonal chains are obtained.

Keywords: Wiener index, expected value, distance, random polygonal chain

AMS Subject classification: 05C12, 05C80, 05C90, 05D40

1 Introduction

All graphs considered in this paper are finite, undirected, connected, without loops and multiple edges. The vertex and edge sets of G are denoted by $V(G)$ and $E(G)$, respectively. If u and v are vertices of G, then the number of edges in the shortest path connecting them is said to be their distance and is denoted by $d(u, v)$. The sum of distances from a vertex v to all vertices in a graph G is called the distance of this vertex, $d(v|G) = \sum_{u \in V(G)} d(u, v)$.

The Wiener index is well-known distance-based topological index introduced by Harold Wiener in 1947 as structural descriptor for acyclic organic molecules. It is defined as the sum of distances between all un-ordered pairs of vertices of a simple graph G, i.e.,

$$W(G) = \sum_{\{u,v\} \subseteq V(G)} d(u, v) = \frac{1}{2} \sum_{v \in V(G)} d(v|G)$$

Mathematical properties and chemical applications of the Wiener index have been intensively studied in the last thirty five years. Nowadays, the Wiener index is one of the best understood and most frequently used molecular shape descriptors. It has found many applications in the modelling of physico-chemical, pharmacological and biological properties of organic molecules. For detailed information on the Wiener index and its applications, we refer to [3–6] and the references cited therein.

Finding explicit expressions for Wiener indices of different classes of polygonal graphs was a focus among the researches concerning the mathematical properties of Wiener index. For example, Gutman [7] investigated the Wiener index of a random benzenoid chains. Bian and Zhang [1] characterize tree-like polyphenyl systems with extremal Wiener indices. Yang and Zhang [8] obtained a formula for the expected value of the Wiener index of a random polyphenyl chain. In addition, Wang et al. [9] also established explicit expressions for the expected value of the Wiener index of three types of random pentagonal chains. Deng [2] gave the recurrences or explicit formulae for computing the Wiener indices of spiro and polyphenyl hexagonal chains and established a relation between the Wiener indices of a spiro hexagonal chain and its corresponding polyphenyl hexagonal chain. Just as showed in [8], polyphenyls themselves and their derivatives have extensive applications in organic synthesis, drug synthesis, heat exchanger, etc. So, it is necessary to study the more general polygonal chains.

Motivated by the works of [7] and [8], the explicit expressions for the expected value of the Wiener indices of two random polygonal chains (see Figures 1-6, whether or not it is chemically realizable) are established in this paper. Although our approach is similar to [7], there are two differences, one is that we take the symmetric properties of the graph into account, this makes the calculation and results more simpler. Another is that our results not only recovered the previous works, but also generalized them. Based on our result, one also can find that the polygonal chains which realize the upper and lower bounds for the Wiener indices of polygonal chains with $n+1$ polygons, this topic usually attract many attentions in the field of chemical graph theory.

The paper is organized as follows. In section 2, we will give two explicit expressions for the expected value of the Wiener indices of two types of random polygonal chains. In section 3, we will provide some applications of our results.

2 The expected value of the Wiener indices of random polygonal chains

In the following, we denote the length of a polygon in a polygonal chain by Δ, the expected value of a random variant X by $E(X)$.

A polygonal chain may be regarded as a graph of linearly concatenated polygons(each of them has the same length Δ), in which the edges connecting polygons share no common vertex. The polygons chain for $n=1$ and $n=2$ are depicted in Figures 1. More generally, a polygonal chain B_n with n polygons (see Figure 2) can be obtained by attaching a polygon to B_{n-1} which has $n-1$ polygons by means of a new edge.

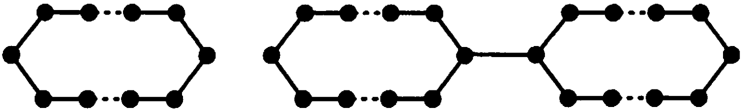

Fig.1. The polygon chains with one and two polygons with $\Delta = 2k$.

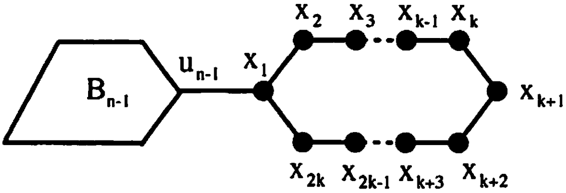

Fig.2. A polygon chain with n polygons and $\Delta = 2k$.

First, we consider the random polygonal chain with $\Delta = 2k$. A random polygonal chain is a polygonal chain obtained by stepwise addition of terminal polygon, we denote it by $R_n^{(1)}$ if it has n polygons with length $\Delta = 2k (k \geq 2)$. Furthermore, at each step $m (3 \leq m \leq n)$ a random selection is made from one of the k possible constructions(see Figure 3, and the superscript i in B_{m+1}^i indicates the distance of the two vertices in the second last polygon with degree 3 is i: (1) $B_m \to B_{m+1}^1$ with probability p_1; (2) $B_m \to B_{m+1}^2$ with probability p_2; $\cdots$; (3) $B_m \to B_{m+1}^{k-1}$ with probability p_{k-1}; (4) $B_m \to B_{m+1}^k$ with probability $1 - p_1 - p_2 - \cdots - p_{k-1}$. Here, we suppose that the process described is a zeroth-order Markov process, which means that the probability $p_1, p_2, \cdots, p_{k-1}$ are constants and independent on the step parameter m.

Theorem 1 The expected value of the Wiener index of the random polygonal chain $R_n^{(1)}$ is

$$E(W(R_{n+1}^{(1)})) = \frac{ka_1}{3}n^3 + 2(k^3 + k^2)n^2 + \frac{1}{3}(9k^3 + 6k^2 - ka_1)n + k^3$$

where

$$a_1 = 2k[2p_1 + 3p_2 + \cdots + kp_{k-1} + (k+1)(1 - p_1 - p_2 - \cdots - p_{k-1})]$$

Proof. As described above, the polygonal chain B_n is constructed by adding a polygon to B_{n-1} by means of a new edge. For this construction, it can be proved that:

1. For any $v \in B_{n-1}$, we have

$$d(x_i, v) = \begin{cases} d(u_{n-1}, v) + i, & \text{if } 1 \leq i \leq k \\ d(u_{n-1}, v) + (2k + 2 - i), & \text{if } k + 1 \leq i \leq 2k. \end{cases}$$

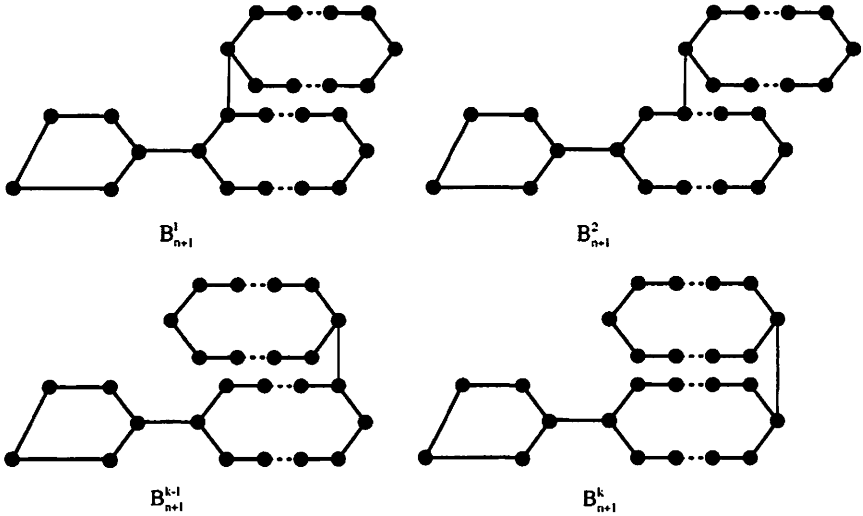

Fig.3. The k types of local arrangements in polygon chains with $\triangle = 2k$.

2. B_{n-1} has $2k(n-1)$ vertices;
3. $\sum_{j=1}^{2k} d(x_i, x_j) = k^2, i \in \{1, 2, \cdots, 2k\}$

From the above relations, one can derive that if $1 \le i \le k$, then

$$d(u_{n-1}|B_{n-1}) + i \times 2k \times (n-1) + k^2, \tag{1}$$

and if $k+1 \le i \le 2k$, then

$$d(u_{n-1}|B_{n-1}) + (2k+2-i) \times 2k \times (n-1) + k^2. \tag{2}$$

It follows that

$$\begin{aligned} W(B_n) &= W(B_{n-1}) + \sum_{i=1}^{2k} \sum_{v \in B_{n-1}} d(x_i, v) + \sum_{1 \le i < j \le 2k} d(x_i, x_j) \\ &= W(B_{n-1}) + \sum_{i=1}^{2k} [d(x_i|B_n) - \sum_{j=1}^{2k} d(x_i, x_j)] + \frac{1}{2} \sum_{i=1}^{2k} \sum_{i=1}^{2k} d(x_i, x_j) \\ &= W(B_{n-1}) + 2kd(u_{n-1}|B_{n-1}) + 2k(k^2+2k)n - (k^3+4k^2) \end{aligned} \tag{3}$$

with the boundary condition $W(B_0) = d(u_0|B_0) = 0$. By substituting n by $n+1$, we have

$$W(B_{n+1}) = W(B_n) + 2kd(u_n|B_n) + 2k(k^2+2k)n + k^3 \tag{4}$$

For a random chain $R_n^{(1)}$, the distance number $d(u_n|R_n^{(1)})$ is a random variable and we denote its expected value by

$$U_n = E(d(u_n|R_n^{(1)}))$$

There are k cases to consider for the random variable $d(u_n|R_n^{(1)})$:
Case 1. $B_n \longrightarrow B_{n+1}^1$. In this case, the vertex u_n coincides with the vertex labeled x_2 or x_{2k}, then, $d(u_n|B_n)$ is given by Eq.(1)with $i = 2$.
Case 2. $B_n \longrightarrow B_{n+1}^2$. In this case, the vertex u_n coincides with the vertex labeled x_3 or x_{2k-1}, then, $d(u_n|B_n)$ is given by Eq.(1) with $i = 3$.
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Case $k-1$. $B_n \longrightarrow B_{n+1}^{k-1}$. In this case, the vertex u_n coincides with the vertex labeled x_k or x_{k+2}, then, $d(u_n|B_n)$ is given by Eq.(1) with $i = k$.
Case k. $B_n \longrightarrow B_{n+1}^k$. In this case, the vertex u_n coincides with the vertex labeled x_{k+1} , then, $d(u_n|B_n)$ is given by Eq.(2) with $i = k+1$.

Since the above k cases occur with probabilities p_1,p_2, $\cdots$, p_{k-1} and $1 - p_1 - p_2 - \cdots - p_{k-1}$, respectively, we have

$$\begin{aligned} U_n = {} & p_1[d(u_{n-1}|R_{n-1}^{(1)}) + 2 \cdot 2k \cdot (n-1) + k^2] + p_2[d(u_{n-1}|R_{n-1}^{(1)}) + 3 \cdot 2k \\ & \cdot (n-1) + k^2] + \cdots + p_{k-1}[d(u_{n-1}|R_{n-1}^{(1)}) + k \cdot 2k \cdot (n-1) + k^2] \\ & + (1 - p_1 - \cdots - p_{k-1})[d(u_{n-1}|R_{n-1}^{(1)}) + (k+1) \cdot 2k \cdot (n-1) + k^2] \end{aligned} \tag{5}$$

by taking the expectation operator to Eq.(5), the recursion formula for U_n can be written in the form of

$$U_n = U_{n-1} + a_1 n + b_1 \tag{6}$$

where

$$a_1 = 2k[2p_1 + 3p_2 + \cdots + kp_{k-1} + (k+1)(1 - p_1 - p_2 - \cdots - p_{k-1})], b_1 = k^2 - a_1$$

with the boundary condition

$$U_0 = E(d(u_0|R_0^{(0)})) = 0 \tag{7}$$

Eq.(6) and Eq.(7) imply that

$$U_n = \frac{a_1}{2} n^2 + (\frac{a_1}{2} + b_1) n \tag{8}$$

By applying the expectation operator to equation (4), and bearing Eq.(8) in mind, we get

$$E(W(R_{n+1}^{(1)})) = E(W(R_n^{(1)})) + k a_1 n^2 + (k b_1 + 3k^3 + 4k^2) n + k^3$$

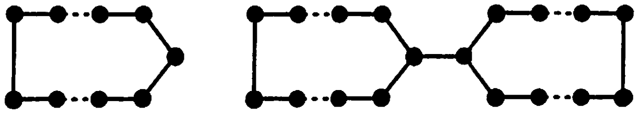

Fig.4. The polygon chains with one and two polygons with $\Delta = 2k+1$.

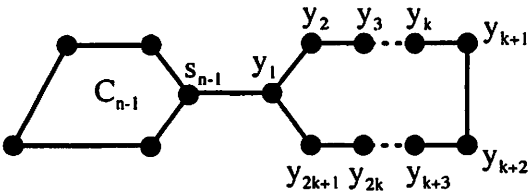

Fig.5. A polygon chains with n polygons and $\Delta = 2k+1$.

with the boundary condition $E(W(R_0^{(0)})) = 0$. The above recurrence relation and boundary condition establish that

$$E(W(R_{n+1}^{(1)})) = \frac{ka_1}{3}n^3 + 2(k^3+k^2)n^2 + \frac{1}{3}(9k^3+6k^2-ka_1)n + k^3$$

which completes the proof of Theorem 1. □

Next, we consider the random polygonal chain with $\Delta = 2k+1$ (see Figures 4-6).

We use $R_{n+1}^{(2)}$ to denote a random polygon chain whose construction just like $R_{n+1}^{(1)}$, the only difference between them is that the length of each polygon changes from $2k$ to $2k+1 (k \geq 1)$.

Theorem 2 The expected value of the Wiener index of the random polygonal chain $R_n^{(2)}$ is

$$\begin{aligned} E(W(R_{n+1}^{(2)})) =& \frac{(2k+1)a_2}{6}n^3 + \frac{1}{2}(4k^3+10k^2+6k+1)n^2 + \frac{1}{6}[18k^3+ \\ & 39k^2+21k+3-(2k+1)a_2]n + \frac{(2k+1)(k^2+k)}{2} \end{aligned} \quad (9)$$

where $a_2 = (2k+1)[k+1-(k-1)p_1-(k-2)p_2-\cdots-p_{k-1}]$.

Proof. The following relations follow from the construction of the polygon chain C_n, which is similar to B_n, see Figures 4-6.

1. For any $w \in C_{n-1}$, we have
$$d(y_i, v) = \begin{cases} d(s_{n-1}, w) + i, & \text{if } 1 \leq i \leq k, \\ d(s_{n-1}, w) + (2k+2-i), & \text{if } k+1 \leq i \leq 2k. \end{cases}$$
2. C_{n-1} has $(2k+1)(n-1)$ vertices;
3. $\sum_{j=1}^{2k+1} d(y_i, y_j) = k^2+k, \quad i \in \{1, 2, \cdots, 2k, 2k+1\}$.

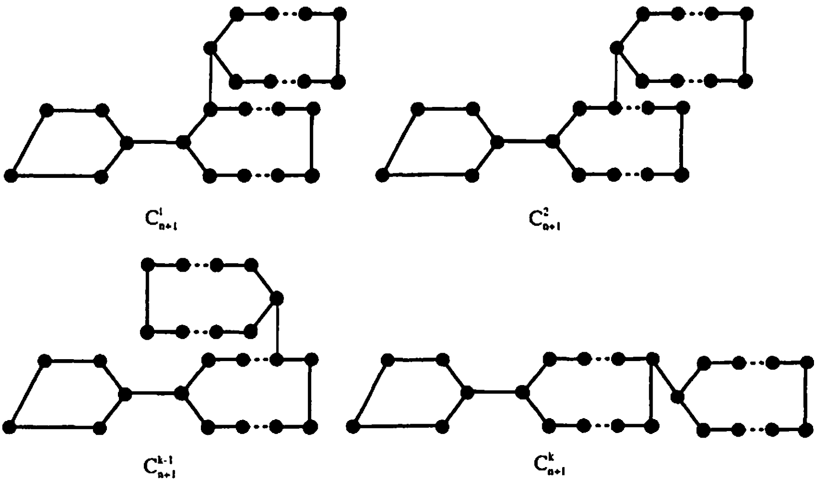

Fig.6. The k types of local arrangements in polygon chains with $\Delta = 2k + 1$.

Hence we have if $k + 1 \leq i \leq 2k$, then

$$d(y_i|C_n) = d(s_{n-1}|C_{n-1}) + i \times (2k+1) \times (n-1) + k^2 + k$$

and if $k + 1 \leq i \leq 2k$, then

$$d(s_{n-1}|C_{n-1}) + (2k + 2 - i) \times (2k+1) \times (n-1) + k^2 + k$$

It follows that

$$W(C_n) = W(C_{n-1}) + (2k+1)d(s_{n-1}|C_{n-1}) + (2k+1) \times [(k+2)(k+1) - 1](n-1) + \frac{(2k+1)(k^2+k)}{2} \quad (10)$$

with the boundary condition $W(C_0) = d(s_0|C_0) = 0$. By replacing n by $n + 1$, Eq.(10) becomes

$$W(C_{n+1}) = W(C_n) + (2k+1)d(s_n|C_n) + (2k+1) \times [(k+2)(k+1) - 1]n + \frac{(2k+1)(k^2+k)}{2}$$

Eq.(9) can be obtained in a similar way as Theorem 1, so we omit the rest of the proof. □

3 Applications

By using Theorems 1 and 2, one can find that the expected value of the Wiener index of some familiar classes of random polygonal chains and the corresponding extremal value.

1. For $\Delta = 6$, the expected value of the Wiener index of random polyphenyl chains can be found by Theorem 1

$$E(W(R_{n+1}^{(1)})) = (24 - 12p_1 - 6p_2)n^3 + 72n^2 + (75 + 12p_1 + 6p_2)n + 27 \quad (11)$$

Eq.(11) has been reported by Yang and Zhang in [8]. If we express it as

$$E(W(R_{n+1}^{(1)})) = 24n^3 + 72n^2 + 75n + 27 + (12p_1 + 6p_2)n(-n^2 + 1)$$

then we can obtain the maximum value and the minimum value of the Wiener index among all polyphenyl chains with $n + 1$ polygons at $p_1 = 0, p_2 = 0$ and $p_1 = 1, p_2 = 0$, respectively, and the corresponding graphs are polyphenyl ortho- and para-chains in [2], respectively.

2. For $\Delta = 5$, the expected value of the Wiener index of random pentagonal chains can be found by Theorem 2

$$E(W(R_{n+1}^{(2)})) = \frac{25}{6}(3 - p_1)n^3 + \frac{85}{2}n^2 + \frac{1}{6}(270 + 25p_1)n + 15 \quad (12)$$

which was found recently in [9]. Similarly, Eq.(12) can be rearranged as

$$E(W(R_{n+1}^{(2)})) = \frac{25}{2}n^3 + \frac{85}{2}n^2 + 30n + 15 + \frac{25}{6}p_1 n(-n^2 + 1)$$

the maximum value and the minimum value of the Wiener index among all pentagonal chains with $n + 1$ polygons at $p_1 = 0$ and $p_1 = 1$, respectively.

3. For $\Delta = 7$, the expected value of the Wiener index of random heptagonal chains can be found by Theorem 2

$$E(W(R_{n+1}^{(2)})) = \frac{49}{6}(4 - 2p_1 - p_2)n^3 + \frac{253}{2}n^2 + \frac{1}{6}(707 + 98p_1 + 49p_2)n + 42 \quad (13)$$

To the best of our knowledge, the result is new for heptagon chains. Eq.(13) implies that

$$E(W(R_{n+1}^{(2)})) = \frac{98}{3}n^3 + \frac{253}{2}n^2 + \frac{707}{6}n + 42 + \frac{49}{6}(2p_1 + p_2)n(-n^2 + 1)$$

the maximum value and the minimum value of the Wiener index among all heptagonal chains with $n+1$ polygons at $p_1 = 0, p_2 = 0$ and $p_1 = 1, p_2 = 0$, respectively.

3. From Theorems 1 and 2, the asymptotic behaviors of $E(W(R^{(1)}_{n+1}))$ and $E(W(R^{(2)}_{n+1}))$ are given by

$$E(W(R^{(1)}_{n+1})) \sim \frac{2k^2}{3}[2p_1 + 3p_2 + \cdots + kp_{k-1} + (k+1)(1 - p_1 - p_2 - \cdots - p_{k-1})]n^3$$

$$E(W(R^{(2)}_{n+1})) \sim \frac{(2k+1)^2}{6}[k + 1 - (k-1)p_1 - (k-2)p_2 - \cdots - p_{k-1}]n^3$$

respectively, for $n \to \infty$, which are cubic in n.

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