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Enumeration of Wiener indices in random polygonal chains

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ABSTRACT

The Wiener index of a connected graph (molecule graph) G is the sum of the distances between all pairs of vertices of G, which was reported by Wiener in 1947 and is the oldest topological index related to molecular branching. In this paper, simple formulae of the expected value of the Wiener index in a random polygonal chain and the asymptotic behavior of this expectation are established by solving a difference equation. Based on the results above, we obtain the average value of the Wiener index of all polygonal chains with n polygons. As applications, we use the unified formulae to obtain the expected values of the Wiener indices of some special random polygonal chains which were deeply discussed in the context of organic chemistry or statistical physics.

1. Introduction

All graphs considered in this paper are simple, undirected and connected. All notation not defined in this paper can be found in the book [7]. Let G be a graph with the vertex set $V(G) = \{v_1, v_2, \ldots, v_n\}$ and edge set $E(G)$. The distance $d(v_r, v_s)$ between vertices v_r and v_s is the number of edges of a shortest path connecting these vertices in G. It is obvious that $d(v_r, v_r) = 0$.

The Wiener index $W(G)$ [21,39] of a graph G was first reported by Wiener in the study of paraffin boiling points and a graph invariant based on distances in 1947. It is defined as the sum of distances between all pairs of vertices in G, i.e.,

$$W(G) = \sum_{r<s} d(v_r, v_s) = \frac{1}{2}\sum_{r=1}^{n} d(v_r|G),$$

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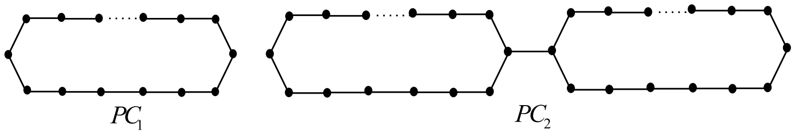

Fig. 1. The polygonal chains for $n = 1$ and $n = 2$.

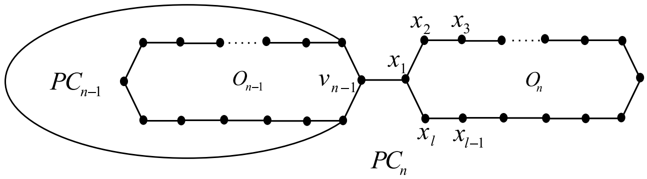

Fig. 2. An l-polygonal chain PC_n with n polygons, where O_n is an l-cycle.

where $d(v_r|G)$ denotes the sum of distances between v_r and all other vertices of G defined by

$$d(v_r|G) = \sum_{s=1}^{n} d(v_r, v_s).$$

The Wiener index is the oldest topological index related to molecular branching [34]. A tentative explanation of the relevance of the Wiener index in research of QSPR and QSAR is that it correlates with the van der Waals surface area of the molecule [19]. In the second half of the 20th century, the Wiener index was found to be correlated with many physico-chemical properties and to have pharmacologic applications. Chen et al. [10,11] considered the problem of the Wiener index in the catacondensed hexagonal systems and investigate the relationships between the Wiener index and other distance-based topological indices in the tree-like polyphenyl systems in 2016. Shiu et al. [28–32] determined the Wiener indices of some pericondensed hexagonal systems. For a survey of results and further bibliography on the chemical applications and the mathematical literature of the Wiener index, see [13–15,40] and the references cited therein.

A polygonal chain of n cycles (polygons) is obtained from a sequence of cycles, $O_1, O_2, \ldots, O_n$, by adding a bridge to each pair of consecutive cycles. If all such cycles are l-cycles, then this polygonal chain is called an *l-polygonal chain* (*of length n*) and denoted by PC_n. The cycle O_i will be called the *i-th polygon* of PC_n, $1 \le i \le n$. Fig. 1 shows the unique polygonal chains for $n = 1$ and $n = 2$, and Fig. 2 shows a general case, where v_{n-1} is a vertex of O_{n-1} in PC_{n-1}. Note that, there are many ways to add a bridge between two consecutive cycles. So PC_n may not be unique when $n \ge 3$. But PC_n is unique when $n = 1, 2$ (see Fig. 1).

Consider PC_{n-1} for $n \ge 3$. Let $O_{n-1} = x_1x_2 \cdots x_lx_1$ and there is a bridge connecting x_1 and v_{n-2} which is a vertex in O_{n-2}. Let $k = \lfloor \frac{l}{2} \rfloor$. By symmetry, there are k ways to add a bridge between the $(n-1)$-st cycle O_{n-1} of PC_{n-1} to the extra l-cycle O_n. Precisely, let PC_n^i be obtained by adding a bridge connecting a vertex of the extra l-cycle O_n with the vertex x_{i+1} of O_{n-1} (see Fig. 3), where $1 \le i \le k$. We may assume that for getting a PC_n from a fixed PC_{n-1} is a random process. Namely, the probability of getting PC_n^i from a fixed PC_{n-1} is p_i. Of course $\sum\limits_{i=1}^{k} p_i = 1$.

We assume that the probabilities $p_1, p_2, \ldots, p_k$ are constants and independent of n, i.e., the process described above is a zeroth-order Markov process. After associating probabilities, such an l-polygonal chain is called a *random l-polygonal chain* and denoted by $PC(n; p_1, p_2, \ldots, p_k)$. Gutman et al. [19,20] considered the Wiener indices of random benzenoid chain graphs in 1990s. Bian and Zhang [6] discussed the Wiener indices of tree-like polyphenyl systems. Chen and Zhang [9] obtained the explicit analytical expressions for the expected values of the Wiener index and the number of perfect matchings in a random phenylene chain. Yang and Zhang [40] studied the Wiener indices of random polyphenyl chains (i.e. 6-polygonal chains) in 2012. Wang et al. [35] considered the problem of the Wiener indices of random pentagonal chains (i.e.,