The Variance, Skewness and Limiting Behavior of the Wiener Index for Random Pentagonal Chain

Priyanka Agarwal¹, Ankur Bharali²

Department of Mathematics, Dibrugarh University, Dibrugarh, 786004.Assam, India

Muran Cancan³

Faculty of Education, Van Yuzuncu Yıl University, Zeve Campus, Tuşba, 65080, Van, Turkey Mohammad Reza Farahani⁴, Mehdi Alaeiyan⁵

Department of Mathematics, Iran University of Science and Technology, Narmak, Tehran 16844, Iran. E-mail: priyanka.agarwal0012@gmail.com, a.bharali@dibru.ac.in (Corresponding author), mcancan@yyu.edu.tr, m_cencen@yahoo.com, mrfarahani88@gmail,com, alaeiyan@iust.ac.ir (0000-0002-5379-2596, 0000-0001-8642-3933, 0000-0002-8606-2274, 0000-0003-2969-4280, 0000-0003-2185-

5967)

Issue: Special Issue on Mathematical Computation in Combinatorics and Graph Theory in Mathematical Statistician and Engineering Applications	Abstract The network graph is a tool to study various complex systems in real world situations such as social networks, food webs, internet etc. In this work, we study the statistical parameters of the random pentagonal chain network, PG_n like dispersion and asymmetry. We establish the explicit
Article Info Page Number: 25 - 37 Publication Issue: Vol 71 No. 3s3 (2022)	formulas for the expected value, variance and skewness of the Wiener index. Further, we obtain that the index obeys normal distribution asymptotically. Keywords : Wiener index, Random Pentagonal Chain, Expected value, Variance, Skewness, Normal distribution.
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1. Introduction

The theory of complex networks [14, 19] is encouraged by experiential or observed phenomena of real networks. One of the basic and most effective tool to study the complex networks or random networks/chains is the theory of graph. The advantage to model the networks to a graph reduces the intricacy of the problem in a practical way and become more tractable. Nowadays, complex networks have become an utmost area in scientific research, especially in the field of statistics, mathematics, physics, chemistry and information science.

Topological index is a numerical value associated with the chemical structure which investigate the related properties and connected informations [1, 9, 11, 13, 23]. In recent years, there exist a legion of topological indices in the literature. Suppose G represents a simple undirected graph with vertex set V(G) and edge set E(G) [3, 7]. The degree of the vertex v is denoted by d(v). The length of the shortest path between any two vertices u and v represents the distance between the vertices u and v, denoted by d(u, v). The Wiener index W(G), introduced by Wiener [22] in 1947, is the first distance based topological index which has many applications and high correlations with physicochemical properties of the molecular compounds. W(G) is the sum of the distances between all pairs of vertices in a graph G, denoted by

$$W(G) = \sum_{\{u,v\}\subseteq V_G} d(u,v) \ (1.1)$$

Yang and Zhang [24] and Ma et al. [12] obtained explicit formulas of W(G) and E(W(G)) for a class of random hexagonal chain networks, respectively. In 2016, Chen et al. studied the relationships between the Wiener index and other distance- based topological indices in the tree – like polyphenyl systems. In 2020, Alaeiyan et al. [2] obtained the exact formulas for the Wiener polarity index of nanostar dendrimers. Due to high correlation of Wiener index with the physicochemical properties of the compounds, researchers from mathematics, statistics and chemistry were more attracted. For more applications of this index, interested readers can refer to [4-6, 10, 16-18, 20, 21, 27-36].

A random pentagonal chain networks are finite 2-connected graphs composed by connecting edges at the ends of the pentagons. A pentagonal chain PG_n with *n* pentagons is obtained by connecting a new pentagon randomly by an edge to a pentagonal chain PG_{n-1} as shown in Fig 2. The pentagonal chains for n = 1, 2, 3 are shown in Fig 1. However, for $n \ge 3$, there are two ways of attaching terminal pentagons which are describes as PG_n^1 and PG_n^2 , as shown in Fig 3. At each step for k = 3, 4, ..., n, the random chain is stochastic and let us choose one of the two possibilities :

(i) $PG_{k-1} \rightarrow PG_k^1$ with probability p_1 ,

(ii) $PG_{k-1} \rightarrow PG_k^2$ with probability $p_2 = 1 - p_1$,

where p_1 and p_2 are constants and steady with the parameter k.

Motivated by [25, 26], Z_n^1 and Z_n^2 are two random variables to represent our choices. If our choice is PG_n^i , we put $Z_n^i = 1$, otherwise $Z_n^i = 0$ (i = 1, 2). One holds that

 $P(Z_n^i = 1) = p_i, P(Z_n^i = 0) = 1 - p_i, i = 1, 2$ (1.2) and $Z_n^1 + Z_n^2 = 1.$

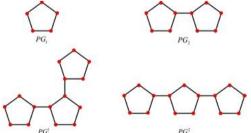


Figure 1. Three types of random chain networks.

The set of statistical parameters to measure a distribution are called moments. There are some more measures apart from central value and dispersion which are *skewness* and *kurtosis*. Skewness(μ_3) refers to lack of symmetry or which describes asymmetry. The importance of the concept of skewness is based upon the assumption of the normal distributions.

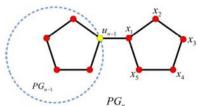


Figure 2. A random chain networks PG_n

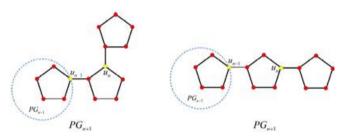


Figure 3. The two types of local arrangements in random chain networks

In this article, we determine the explicit formulas of $E(W(PG_n)), Var(W(PG_n))$ and $\mu_3(W(PG_n))$ of random chain based on some known results. Furthermore, asymptotic behavior of expected value of Wiener index is also considered and prove that the random variable $W(PG_n)$ asymptotically obey normal distributions.

For this results, we must ensure that the following Hypothesis hold.

Hypothesis 1. It is randomly and independently to choice a way attaching the new terminal pentagon O_{n+1} to $PG_n, n = 2, 3, ...$ To be more precisely, the sequences of random variables $\{Z_n^1, Z_n^2\}_{n=2}^{\infty}$ are independently and must satisfy Eq. (1.2).

Hypothesis 2. *For* $i \in \{1, 2\}$ *, we put* $0 < p_i < 1$ *.*

Under the conditions of Hypothesis 1 and 2.

(a)The analytical expressions of the variance and skewness of $W(PG_n)$ are obtained;

(b)When $n \to \infty$, we verify that the random variable $W(PG_n)$ asymptotically obey normal distributions. It is evident to see that

$$\lim_{n \to \infty} \sup_{a \in \mathbf{R}} \left| \mathbf{P}\left(\frac{X_n - E(X_n)}{\sqrt{Var(X_n)}} \le a\right) - \int_{-\infty}^a \frac{1}{\sqrt{2\pi}} e^{\frac{-z^2}{2}dz} \right| = 0$$

where $E(X_n)$ and $Var(X_n)$ represent the expectation and variance of this random variable X_n , respectively.

In this paper, assume that f(x) and g(x) are two functions of x. Then

(i)
$$f(x) \approx g(x)$$
 if $\lim_{x \to \infty} \frac{f(x)}{g(x)} = 1$.
(ii) $f(x) = O(g(x))$ if $\lim_{x \to \infty} \frac{f(x)}{g(x)} = 0$.

2. Results

For the random chain networks PG_n , $W(PG_n)$ is the random variable. Here, we determine the explicit formulas of $E(W(PG_n))$, $Var(W(PG_n))$ and $\mu_3(W(PG_n))$. In addition, we show the asymptotic behavior of expected value and prove the index obeys normal distributions asymptotically.

In fact, PG_n is obtained by adding a new terminal pentagon O_n to PG_{n-1} by an edge, where x_1, x_2, x_3, x_4, x_5 are the vertices of O_n arranged in clockwise direction. For all $v \in V_{PG_{n-1}}$, we have

1. $d(x_1, v) = d(u_{n-1}, v) + 1, d(x_2, v) = d(u_{n-1}, v) + 2,$ $d(x_3, v) = d(u_{n-1}, v) + 3, d(x_4, v) = d(u_{n-1}, v) + 3, \text{ and } d(x_5, v) = d(u_{n-1}, v) + 2.$ 2. PG_{n-1} has 5(n-1) vertices. 3. $\sum_{i=1}^{5} d(x_k, x_i) = 6, \forall k = 1, 2, 3, 4, 5.$

Theorem 2.1: For $n \ge l$, the analytic expression of $E(W(PG_n))$ for the random chain networks is

$$E(W(PG_n)) = \frac{5}{6} (15 - 5p_1)n^3 + \frac{1}{2} (25p_1 + 10)n^2 - \frac{1}{6} (50p_1 + 15)n$$

Proof: By Eq. (1.1), we have $W(PG_{n+1}) = \sum_{\{u,v\} \subseteq V_{PG_n}} d(u,v) + \sum_{v \in V_{PG_n}} \sum_{x_i \in V_{O_{n+1}}} d(v, x_i) + \sum_{\{x_i, x_j\} \subseteq V_{O_{n+1}}} d(x_i, x_j)$ $= W(PG_n) + \sum_{v \in V_{PG_n}} (5d(u_n, v) + 11) + \frac{1}{2} \sum_{i=1}^5 \sum_{j=1}^5 d(x_i, x_j)$ $= W(PG_n) + 5 \sum_{v \in V_{PG_n}} d(u_n, v) + 55n + 15 (2.1)$

For the random chain networks PG_n , we obtain that $\sum_{v \in V_{PG_n}} d(u_n, v)$ is a random variable. Let

$$A_n = E\left(\sum_{v \in V_{PG_n}} d(u_n, v)\right).$$

By using the above formula and Eq. (2.1), $E(W(PG_{n+1}))$ of the random chain network is $E(W(PG_{n+1})) = E(W(PG_n)) + 5A_n + 55n + 15$ (2.2)

Then, the following two cases arise:

Case 1. $PG_n \rightarrow PG_{n+1}^1$.

In this case, u_n (of PG_n) coincides with the vertex labeled x_2 or x_5 (of O_n). Therefore, $\sum_{v \in V_{PG_n}} d(u_n, v)$ can be written as $\sum_{v \in V_{PG_n}} d(x_2, v)$ or $\sum_{v \in V_{PG_n}} d(x_5, v)$ with probability p_1 . **Case 2.** $PG_n \rightarrow PG_{n+1}^2$.

In this case, u_n (of PG_n) coincides with the vertex labeled x_3 or x_4 (of O_n). Therefore, $\sum_{v \in V_{PG_n}} d(u_n, v)$ can be written as $\sum_{v \in V_{PG_n}} d(x_3, v)$ or $\sum_{v \in V_{PG_n}} d(x_4, v)$ with probability $p_2 = 1 - p_1$.

By applying the expectation operator together with the above cases,

$$A_n = p_1 \sum_{v \in V_{PG_n}} d(x_2, v) + p_2 \sum_{v \in V_{PG_n}} d(x_3, v)$$

where

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$$\sum_{v \in V_{PG_n}} d(x_2, v) = \sum_{v \in V_{PG_{n-1}}} (d(u_{n-1}, v) + 2) + \sum_{v \in O_n} d(x_2, v)$$
$$= \sum_{v \in V_{PG_{n-1}}} d(u_{n-1}, v) + 10(n-1) + 6.$$
$$\sum_{v \in V_{PG_n}} d(x_3, v) = \sum_{v \in V_{PG_{n-1}}} (d(u_{n-1}, v) + 3) + \sum_{v \in O_n} d(x_3, v)$$
$$= \sum_{v \in V_{PG_{n-1}}} d(u_{n-1}, v) + 15(n-1) + 6.$$

Then, we obtain

$$\begin{split} A_n &= p_1 \left[\sum_{v \in V_{PG_n}} d(u_{n-1}, v) + 10(n-1) + 6 \right] + (1-p_1) \left[\sum_{v \in V_{PG_{n-1}}} d(u_{n-1}, v) + 15(n-1) + 6 \right] \\ &= A_{n-1} + p_1(10n-4) + (1-p_1)(15n-9) \\ &= A_{n-1} + (15-5p_1)n + (-9+5p_1). \end{split}$$
 For $n = 1$, the boundary condition is

$$A_1 = E\left(\sum_{v \in V_{PG_1}} d(u_1, v)\right) = 6.$$

Using the above condition and recurrence relation with respect to A_n ,

$$A_n = \left(\frac{15}{2} - \frac{5}{2}p_1\right)n^2 + \left(\frac{5}{2}p_1 - \frac{3}{2}\right)n. (2.3)$$

From Eq. (2.2), it holds that

 $E(W(PG_{n+1})) = E(W(PG_n)) + 5A_n + 55n + 15$ = $E(W(PG_n)) + 5\left[\left(\frac{15}{2} - \frac{5}{2}p_1\right)n^2 + \left(\frac{5}{2}p_1 - \frac{3}{2}\right)n\right] + 55n + 15.$

For n = 1, we obtain $E(W(PG_1)) = 15$. Similarly, according to the recurrence relation related to $E(W(PG_n))$, we have

$$E(W(PG_n)) = \frac{5}{6} (15 - 5p_1)n^3 + \frac{1}{2} (25p_1 + 10)n^2 - \frac{1}{6} (50p_1 + 15)n^3$$

Also,

$$E(W(PG_n)) \sim \frac{5}{6} (15 - 5p_1)n^3.$$

i.e. $E(W(PG_n))$ is asymptotic to a cubic in n as $n \to \infty$.

Theorem 2.2: Suppose Hypothesis 1 and 2 are correct, then the variance of the Wiener index is denoted by

$$Var(W(PG_n)) = \frac{1}{30}(v_1n^5 - 5r_1n^4 + 10v_2n^3 + (65r_1 - 30v_1 - 45v_2)n^2 + (59v_1 + 65v_2 - 120r_1)n + (60r_1 - 30v_1 - 30v_2)).$$

where

$$(U_m) = v_1, Var(V_m) = v_2, Cov(U_m, V_m) = r_1.$$

Proof: Let $B_n = 5 \sum_{v \in V_{PG_n}} d(u_n, v)$. Then by Eq. (2.1), we obtain

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$$W(PG_{n+1}) = W(PG_n) + B_n + 55n + 15$$
(2.4)

Recalling that Z_n^1 and Z_n^2 are random variables for the choice to construct PG_{n+1} by PG_n . Now the next two facts are:

Fact 1 $B_n Z_n^1 = (B_{n-1} + 50n - 20)Z_n^1$.

Proof. If $Z_n^1 = 0$, it is obvious. Then we only take into account $Z_n^1 = 1$, which implies $PG_n \rightarrow PG_{n+1}^1$. In this case, u_n coincides with x_2 or x_5 , see Fig 3.

$$\begin{split} B_n &= 5 \sum_{v \in V_{PG_n}} d(x_2, v) \\ &= 5 \sum_{v \in V_{PG_{n-1}}} d(x_2, v) + 5 \sum_{v \in V_{O_n}} d(x_2, v) \\ &= 5 \sum_{v \in V_{PG_{n-1}}} (d(u_{n-1}, v) + d(u_{n-1}, x_2)) + 30 \\ &= B_{n-1} + 50n - 20. \\ \text{Thus, we conclude the desired fact.} \\ \mathbf{Fact } 2 B_n Z_n^2 &= (B_{n-1} + 75n - 45) Z_n^2. \\ \text{Similarly, by taking into account } PG_n \to PG_{n+1}^2, \text{ we get the Fact } 2. \\ \text{Notice that } Z_n^1 + Z_n^2 &= 1, \text{ from the above two facts, it holds that} \\ B_n &= B_n (Z_n^1 + Z_n^2) \\ &= (B_{n-1} + 50n - 20) Z_n^1 + (B_{n-1} + 75n - 45) Z_n^2 \\ &= B_{n-1} + (50Z_n^1 + 75Z_n^2)n - (20Z_n^1 + 45Z_n^2) \\ &= B_{n-1} + nU_n - V_n \\ \text{where for each } n, \\ U_n &= 50Z_n^1 + 75Z_n^2, V_n &= 20Z_n^1 + 45Z_n^2. \\ \text{Therefore, by Eq. } (2.4), \text{ it follows that} \\ W(PG_n) &= W(PG_1) + \sum_{l=1}^{n-1} (\sum_{m=1}^{l-1} (B_{m+1} - B_m) + B_1) + \sum_{l=1}^{n-1} (55l + 15) \\ &= W(PG_1) + \sum_{l=1}^{n-1} \sum_{m=1}^{l-1} ((m+1)U_{m+1} - V_{m+1}) + O(n^2) (2.5) \\ \text{Pu direct a cloudition, we have,} \end{split}$$

By direct calculation, we have

$$v_{1} = 50^{2}p_{1} + 75^{2}(1 - p_{1}) - (50p_{1} + 75(1 - p_{1}))^{2},$$

$$v_{2} = 20^{2}p_{1} + 45^{2}(1 - p_{1}) - (20p_{1} + 45(1 - p_{1}))^{2},$$

$$r_{1} = 50.20, p_{1} + 75.45, (1 - p_{1}) - (50p_{1} + 75(1 - p_{1}))(20p_{1} + 45(1 - p_{1})).$$

Refer to ref. [25, 26], by the properties of variance, Eq. (2.5) and exchanging the order of l and m, we have directly

$$Var(W(PG_{n})) = Var\left[\sum_{l=1}^{n-1}\sum_{m=1}^{l-1}((m+1)U_{m+1} - V_{m+1})\right]$$

$$= Var\left[\sum_{m=1}^{n-2}\sum_{l=m+1}^{n-1}((m+1)U_{m+1} - V_{m+1})\right]$$

$$= Var\left[\sum_{m=1}^{n-2}((m+1)U_{m+1} - V_{m+1})(n - m - 1)\right]$$

$$= \sum_{m=1}^{n-2}(n - m - 1)^{2}Var((m+1)U_{m+1} - V_{m+1})$$

$$= \sum_{m=1}^{n-2}(n - m - 1)^{2}Cov((m+1)U_{m+1} - V_{m+1}, (m+1)U_{m+1} - V_{m+1})$$

$$= \sum_{m=1}^{n-2}(n - m - 1)^{2}((m+1)^{2}Cov(U_{m+1}, U_{m+1}) - 2(m+1)Cov(U_{m+1}, V_{m+1}) + Cov(V_{m+1}, V_{m+1}))$$

$$= \sum_{m=1}^{n-2}(n - m - 1)^{2}((m+1)^{2}v_{1} - 2(m+1)r_{1} + v_{2})$$

By computing, we get the result.

Theorem 2.3: Suppose Hypothesis 1 and 2 are correct, then the skewness of the Wiener index is denoted by

 $\mu_3 (W(PG_n)) = \frac{1}{420} (3s_1 n^7 + (-147r_3 + 294m_1 r_1)n^6 + (63r_2 - 126m_2 r_1) \\ n^5 + (-105s_2 + 210r_3 - 420m_1 r_1)n^4 + (-413s_1 + 630s_2 - 1365r_2 + 1260r_3 - 2520m_1 r_1 + 2730m_2 r_1)n^3 + (1260s_1 - 1365s_2 + 3780r_2 - 63r_3 + 126r_1 - 1365r_2 + 1260r_2 - 1360r_2 - 63r_3 + 126r_1 - 1360r_2 - 1260r_3 - 2520m_1 r_1 \\ -84m_2 r_1)n + (420s_1 - 420s_2 + 1260r_2 - 1260r_3 + 2520m_1 r_1 - 2520m_2 r_1)), where,$

$$E(U_m) = m_1, E(V_m) = m_2, Var(U_m) = v_1, Var(V_m) = v_2, Cov(U_m, V_m) = r_1, Cov(U_m, V_m^2) = r_2, Cov(U_m^2, V_m) = r_3,$$

$$\begin{split} \mu_{3}(U_{m}) &= s_{1}, \mu_{3}(V_{m}) = s_{2}. \\ \textit{Proof:} \text{ By direct calculation, we have} \\ m_{1} &= 50.p_{1} + 75.(1 - p_{1}), \\ m_{2} &= 20.p_{1} + 45.(1 - p_{1}), \\ v_{1} &= 50^{2}p_{1} + 75^{2}(1 - p_{1}) - (50p_{1} + 75(1 - p_{1}))^{2}, \\ v_{2} &= 20^{2}p_{1} + 45^{2}(1 - p_{1}) - (20p_{1} + 45(1 - p_{1}))^{2}, \\ r_{1} &= 50.20.p_{1} + 75.45.(1 - p_{1}) - (50p_{1} + 75(1 - p_{1}))(20p_{1} + 45(1 - p_{1})), \\ r_{2} &= 50.20^{2}.p_{1} + 75.45^{2}.(1 - p_{1}) - (50p_{1} + 75(1 - p_{1}))(20^{2}p_{1} + 45^{2}(1 - p_{1})), \\ r_{3} &= 50^{2}.20.p_{1} + 75^{2}.45.(1 - p_{1}) - (50^{2}p_{1} + 75^{2}(1 - p_{1}))(20p_{1} + 45(1 - p_{1})), \end{split}$$

$$\begin{split} s_1 &= 50^3 \cdot p_1 + 75^3 \cdot (1-p_1) - 3 \big(50^2 p_1 + 75^2 (1-p_1) \big) \cdot \big(50 p_1 + 75 (1-p_1) \big) + 2 \\ (50 p_1 + 75 (1-p_1))^3 , \\ s_2 &= 20^3 \cdot p_1 + 45^3 \cdot (1-p_1) - 3 \big(20^2 p_1 + 45^2 (1-p_1) \big) \cdot \big(20 p_1 + 45 (1-p_1) \big) + 2 \big(20 p_1 + 45 (1-p_1) \big)^3 . \end{split}$$

By the properties of skewness, Eq. (2.5) and exchanging the order of l and m, we have directly

$$\begin{split} &\mu_{3} \Big(W(PG_{n}) \Big) = \mu_{3} \left[\sum_{l=1}^{n-1} \sum_{m=1}^{l-1} \left((m+1)U_{m+1} - V_{m+1} \right) \right] \\ &= \mu_{3} \left[\sum_{m=1}^{n-2} \sum_{l=m+1}^{n-1} \left((m+1)U_{m+1} - V_{m+1} \right) \right] \\ &= \mu_{3} \left[\sum_{m=1}^{n-2} ((m+1)U_{m+1} - V_{m+1})(n-m-1) \right] \\ &= \sum_{m=1}^{n-2} (n-m-1)^{3} \mu_{3} ((m+1)U_{m+1} - V_{m+1}) \\ &= \sum_{m=1}^{n-2} (n-m-1)^{3} \left[E \left(\left((m+1)U_{m+1} - V_{m+1} \right)^{3} \right) - 3E \left(\left((m+1)U_{m+1} - V_{m+1} \right)^{2} \right) \right] \\ &E \left((m+1)U_{m+1} - V_{m+1} \right) + 2 \left(E \left((m+1)U_{m+1} - V_{m+1} \right) \right)^{3} \right] \\ &= \sum_{m=1}^{n-2} (n-m-1)^{3} \left[(m+1)^{3} \mu_{3} (U_{m+1}) - \mu_{3} (V_{m+1}) + 3(m+1)Cov(U_{m+1}, V_{m+1}) \right] \\ &= \sum_{m=1}^{n-2} (n-m-1)^{3} \left[(m+1)^{3} \mu_{3} (U_{m+1}) + 6(m+1)^{2} E(U_{m+1})Cov(U_{m+1}, V_{m+1}) \right] \\ &= \sum_{m=1}^{n-2} (n-m-1)^{3} \left[(m+1)^{3} s_{1} - s_{2} + 3(m+1)r_{2} - 3(m+1)^{2} + 6(m+1)^{2} m_{1} r_{1} \right] \\ &= \sum_{m=1}^{n-2} (n-m-1)^{3} \left[(m+1)^{3} s_{1} - s_{2} + 3(m+1)r_{2} - 3(m+1)^{2} + 6(m+1)^{2} m_{1} r_{1} \right] \\ &= \sum_{m=1}^{n-2} (n-m-1)^{3} \left[(m+1)^{3} s_{1} - s_{2} + 3(m+1)r_{2} - 3(m+1)^{2} + 6(m+1)^{2} m_{1} r_{1} \right] \\ &= \sum_{m=1}^{n-2} (n-m-1)^{3} \left[(m+1)^{3} s_{1} - s_{2} + 3(m+1)r_{2} - 3(m+1)^{2} + 6(m+1)^{2} m_{1} r_{1} \right] \\ &= \sum_{m=1}^{n-2} (n-m-1)^{3} \left[(m+1)^{3} s_{1} - s_{2} + 3(m+1)r_{2} - 3(m+1)^{2} + 6(m+1)^{2} m_{1} r_{1} \right] \\ &= \sum_{m=1}^{n-2} (n-m-1)^{3} \left[(m+1)^{3} s_{1} - s_{2} + 3(m+1)r_{2} - 3(m+1)^{2} + 6(m+1)^{2} m_{1} r_{1} \right] \\ &= \sum_{m=1}^{n-2} (n-m-1)^{3} \left[(m+1)^{3} s_{1} - s_{2} + 3(m+1)r_{2} - 3(m+1)^{2} + 6(m+1)^{2} m_{1} r_{1} \right] \\ &= \sum_{m=1}^{n-2} (n-m-1)^{3} \left[(m+1)^{3} s_{1} - s_{2} + 3(m+1)r_{2} - 3(m+1)^{2} + 6(m+1)^{2} m_{1} r_{1} \right] \\ &= \sum_{m=1}^{n-2} (n-m-1)^{3} \left[(m+1)^{3} s_{1} - s_{2} + 3(m+1)r_{2} - 3(m+1)^{2} + 6(m+1)^{2} m_{1} r_{1} \right] \\ &= \sum_{m=1}^{n-2} (n-m-1)^{3} \left[(m+1)^{3} s_{1} - s_{2} + 3(m+1)r_{2} - 3(m+1)^{2} + 6(m+1)^{2} m_{1} r_{1} \right] \\ &= \sum_{m=1}^{n-2} (n-m-1)^{3} \left[(m+1)^{3} s_{1} - s_{2} + 3(m+1)r_{2} - 3(m+1)^{2} + 6(m+1)^{2} m_{1} r_{1} \right] \\ &= \sum_{m=1}^{n-2} (n-m-1)^{3} \left[(m+1)^{3} s_{1} - s_{2} + 3(m+1)r_{2} - 3(m+1)r$$

By computing, we get the result.

Theorem 2.4: For $n \to \infty$, $W(PG_n)$ asymptotically obeys normal distribution. One has $\lim_{n \to \infty} \sup_{a \in \mathbb{R}} \left| \mathbb{P}(\frac{x_n - E(x_n)}{\sqrt{Var(x_n)}} \le a) - \int_{-\infty}^{a} \frac{1}{\sqrt{2\pi}} e^{\frac{-z^2}{2}dz} \right| = 0.$

Proof: Firstly, for any $n \in N$, let

$$\boldsymbol{U}_{\boldsymbol{n}} = \sum_{l=1}^{n-1} \sum_{m=1}^{l-1} (m+1) U_{m+1}, \, \boldsymbol{V}_{\boldsymbol{n}} = \sum_{l=1}^{n-1} \sum_{m=1}^{l-1} V_{m+1}, \, \varphi(z) = E\left(e^{z(U_m - m_1)}\right).$$

By these notations, we have

$$e^{z(U_n - E(U_n))} = e^{z\sum_{l=1}^{n-1}\sum_{m=1}^{l-1}(m+1)(U_{m+1} - m_1)}$$
$$= e^{z\sum_{m=1}^{n-2}\sum_{l=m+1}^{n-1}(m+1)(U_{m+1} - m_1)}$$

$$=e^{z\sum_{m=1}^{n-2}(n-m-1)(m+1)(U_{m+1}-m_1)}.$$

then

$$E[e^{z(U_n - E(U_n))}] = E[e^{z\sum_{m=1}^{n-2} (n - m - 1)(m + 1)(U_{m+1} - m_1)}]$$

=
$$\prod_{m=1}^{n-2} E(e^{z(n - m - 1)(m + 1)(U_{m+1} - m_1)})$$

=
$$\prod_{m=1}^{n-2} \varphi(z(n - m - 1)(m + 1)), (2.6)$$

and for some k > 0, $V_n = \sum_{l=1}^{n-1} \sum_{m=1}^{l-1} V_{m+1} \le kn^2$. (2.7) Noting that

$$Var(W(PG_n)) \approx \frac{1}{30} v_1 n^5, \varphi(z) = 1 + \frac{v_1}{2} z^2 + O(z^2),$$

and

$$\sum_{m=1}^{n-2} (m+1)^2 (n-m-1)^2 \approx \frac{n^5}{30}$$

By Taylor's formula and Eqs. (2.5)-(2.7), we have

$$\begin{split} &\lim_{n \to \infty} E \, exp \left\{ z \, \frac{W(PG_n) - E(W(PG_n))}{\sqrt{Var(W(PG_n))}} \right\} \\ &= \lim_{n \to \infty} E \, exp \left\{ z \, \frac{\left(W(PG_1) + \mathbf{U}_n - \mathbf{V}_n + O(n^2)\right) - E(W(PG_1) + \mathbf{U}_n - \mathbf{V}_n + O(n^2))\right)}{\frac{\sqrt{v_1}n^{\frac{5}{2}}}{\sqrt{30}}} \right\} \\ &= \lim_{n \to \infty} E \, exp \left\{ z \, \frac{\sqrt{30}(\mathbf{U}_n - E(\mathbf{U}_n))}{\sqrt{v_1}n^{\frac{5}{2}}} \right\} \\ &= \lim_{n \to \infty} \prod_{m=1}^{n-2} \varphi \left(\frac{\sqrt{30}z(m+1)(n-m-1)}{\sqrt{v_1}n^{\frac{5}{2}}} \right) \right\} \\ &= \lim_{n \to \infty} exp \left\{ \sum_{m=1}^{n-2} \ln \varphi \left(\frac{\sqrt{30}z(m+1)(n-m-1)}{\sqrt{v_1}n^{\frac{5}{2}}} \right) \right\} \\ &= \lim_{n \to \infty} exp \left\{ \sum_{m=1}^{n-2} \ln \left(1 + \frac{v_1}{2} \cdot \frac{30z^2(m+1)^2(n-m-1)^2}{v_1n^5} + O\left(\frac{1}{n}\right) \right) \right\} \\ &= \lim_{n \to \infty} exp \left\{ \sum_{m=1}^{n-2} \left(\frac{v_1}{2} \cdot \frac{30z^2(m+1)^2(n-m-1)^2}{v_1n^5} + O\left(\frac{1}{n}\right) \right) \right\} \end{split}$$

$$=e^{\frac{z^2}{2}}.$$

Assume that I is a complex number with $I^2 = 1$. We use Iz instead of z and we get

$$\lim_{n\to\infty} E \exp\left\{Iz\frac{W(PG_n)-E(W(PG_n))}{\sqrt{Var(W(PG_n))}}\right\} = e^{\frac{-z^2}{2}}.$$

Using the above formula ([15], Chapter 1) and probability characteristic functions ([8], Chapter 15), we get the result.

3. Conclusion

There are various complex systems in real world which can be dealt with the network graphs. Gradually, the complex networks is an upsurge to the researchers in the field of statistics, mathematical and information sciences. In recent years, network graphs is very much important to tackle the large complex-systems. In this work, we obtain the expected value, variance and skewness of Wiener index for a class of random chain networks. It is observed that expected value of Wiener index asymptotic to cubic as $n \to \infty$. Moreover, Wiener index for random pentagonal chain approximately obeys normal distribution.

References

- F. Afzal, S. Hussain, D. Afzal, S. Razaq, Some new degree based topological indices via M-polynomial, *Journal of Information and Optimization Sciences*, 41.4, 1061-1076, (2020), https://doi.org/10.1080/02522667.2020.1744307.
- [2] M. Alaeiyan, F. Afzal, M.R. Farahani, M.Ali Rostami, An exact formulas for the Wiener polarity index of nanostar dendrimers, *Journal of Information and Optimization Sciences*, 41(4), 933-939, (2020), https://doi.org/10.1080/02522667.2020.1748274.
- [3] F.-R. King Chung, Spectral Graph Theory, Providence, RI: American Mathematical Society, (1997).
- [4] H. Deng, Wiener indices of spiro and polyphenyl hexagonal chains, *Mathematical and Computer* Modelling, 55.3-4, 634-644, (2012), https://doi.org/10.1016/j.mcm.2011.08.037.
- [5] A.A. Dobrynin, R. Entringer, I. Gutman, Wiener index of trees: theory and applications, *Acta Applicandae Mathematica*, 66, 211-249, (2001), https://doi.org/10.1023/A:1010767517079.
- [6] A.A. Dobrynin, I. Gutman, S. Klavžar, P. Žigert, Wiener index of hexagonal systems, *Acta Applicandae Mathematica*, 72, 247-294, (2002), https://doi.org/10.1023/A:1016290123303.
- [7] R.C. Entringer, D.E. Jackson, D.A. Snyder, Distance in graphs, *Czechoslovak Mathematical Journal*, 26.2, 283-296, (1976), http://dml.cz/dmlcz/101401.
- [8] W. Feller, An introduction to probability theory and its applications, Wiley Series in Probability and Statistics, (1971).

- [9] B. Furtula, I. Gutman, M. Dehmer, On structure-sensitivity of degree-based topological indices, *Applied Mathematics Computation*, 219.17, 8973-8978, (2013), https://doi.org/10.1016/j.amc.2013.03.072.
- [10] W.Gao and M.R. Farahani, The Zagreb topological indices for a type of Benzenoid systems jagged-rectangle, *Journal of Interdisciplinary Mathematics*, 20(5), 1341-1348, (2017), <u>https://doi.org/10.1080/09720502.2016.1232037</u>.
- [11] Pawan Kumar Tiwari, P. S. (2022). Numerical Simulation of Optimized Placement of Distibuted Generators in Standard Radial Distribution System Using Improved Computations. International Journal on Recent Technologies in Mechanical and Electrical Engineering, 9(5), 10–17. https://doi.org/10.17762/ijrmee.v9i5.369
- [12] I. Gutman, Degree based topological indices, *Croatica Chemica Acta*, 86.4, 351-361, (2013), https://dx.doi.org/10.5562/cca2294.
- [13] L. Ma, H. Bian, J.B. Liu, H. Yu, The Expected Values of the Wiener Indices in the Random Phenylene and Spiro Chains, *Ars Combinatoria*, 130, 267-274, (2017).
- [14] M. Nadeem, S. Ahmad, M. K. Siddiqui, M.A. Ali, M.R. Farahani, A.J.M. Khalaf, On some applications related with algebraic structures through different well known graphs, *Journal of Discrete Mathematical Sciences and Cryptography*, 24.2, 451-471, (2021), https://doi.org/10.1080/09720529.2021.1885806.
- [15] M.E. J. Newman, Networks, Oxford University, New York, (2018).
- [16] V.V. Petrov, Limit theorems of probability theory sequences of independent random variables, Oxford University Press, (1995).
- [17] W.C. Shiu, P.C. B. Lam, The Wiener number of the hexagonal net, *Discrete Applied Mathematics*, 73.2, 101-111, (1997), https://doi.org/10.1016/S0166-218X(96)00109-6.
- [18] W.C. Shiu, P.C. B. Lam, Wiener number of pericondensed benzenoid molecule systems, *Congressus Numerantium*, 126, 113-124, (1997).
- [19] W.C. Shiu, C. Tong, P.C. B. Lam, Wiener number of hexagonal jagged-rectangles, *Discrete Applied Mathematics*, 80, 83-96, (1997), https://doi.org/10.1016/s0166-218X(97)00071-1.
- [20] R. Vignesh, K.T. Rajeswari, S. Venkatesh, C. Natarajan, M. Alaeiyan, On some degree-based irregularity indices of certain networks, *Journal of Discrete Mathematical Sciences and Cryptography*, 24.2, 617-628, (2021), https://doi.org/10.1080/09720529.2021.1892269.
- [21] S.Wei, X. Ke, Y. Wang, Wiener indices in random cyclooctane chains, Wuhan University Journal of Natural Sciences, 23, 498-502, (2018), https://doi.org/10.1007/s11859-018-1355-5.
- [22] S. Wei and W.C. Shiu, Enumeration of Wiener indices in random polygonal chains, *Journal of Mathematical Analysis and Applications*, 469.2, 537-548, (2019), https://doi.org/10.1016/j.jmaa.2018.09.027.
- [23] H. Wiener, Structural determination of paraffin boiling points, *Journal of the American Chemical Society*, 69.1, 17-20, (1947), https://doi.org/10.1021/ja01193a005.

- [24] K. Xu, M. Liu, K.C. Das, I. Gutman, B. Furtula, A survey on graphs extremal with respect to distance-based topological indices, *MATCH Communications in Mathematical and in Computer Chemistry*, 71, 461-508, (2014).
- [25] W. Yang, F. Zhang, Wiener Index in Random Polyphenyl Chains, *MATCH Communications in Mathematical and in Computer Chemistry*, 68.1, 371-376, (2018).
- [26] J. Zhang, X. Peng, H. Chen, The limiting behaviours for the Gutman index, Schultz Index, multiplicative degree-Kirchhoff index and additive degree-Kirchhoff index of a random polyphenylene chain, Discrete Applied Mathematics, 299, 62-73, (2021), https://doi.org/10.1016/j.dam.2021.04.016.
- [27] L. Zhang, Q. Li, S. Li, M. Zhang, The expected values for the Gutman index, Schultz Index, multiplicative degree-Kirchhoff index and additive degree-Kirchhoff index of a random polyphenylene chain, Discrete Applied Mathematics, 282, 243-256, (2020), https://doi.org/10.1016/j.dam.2019.11.007.
- [28] Q. Zhou, L. Wang, Y. Lu, Wiener Index and Harary Index on Hamilton-Connected Graphs with Large Minimum Degree, Discrete Applied Mathematics, 247, 180-185, (2018), https://doi.org/10.1016/j.dam.2018.03.063.
- [29] W. Gao, M.R. Rajesh Kanna, E Suresh, M.R. Farahani. Calculating of degree-based topological indices of nanostructures Geology, Ecology, and Landscapes 1 (3), 173-183, 2017.
- [30] W. Gao, M.R. Farahani, S. Wang, M.N. Husin. On the edge-version atom-bond connectivity and geometric arithmetic indices of certain graph operations. Applied Mathematics and Computation 308(1), 11-17, 2017. <u>https://doi.org/10.1016/j.amc.2017.02.046</u>
- [31] Alaria, S. K., A. . Raj, V. Sharma, and V. Kumar. "Simulation and Analysis of Hand Gesture Recognition for Indian Sign Language Using CNN". International Journal on Recent and Innovation Trends in Computing and Communication, vol. 10, no. 4, Apr. 2022, pp. 10-14, doi:10.17762/ijritcc.v10i4.5556.
- [32] H. Wang, JB Liu, S. Wang, W. Gao, S. Akhter, M. Imran, M.R. Farahani. Sharp bounds for the general sum-connectivity indices of transformation graphs. Discrete Dynamics in Nature and Society 2017. Article ID 2941615 | https://doi.org/10.1155/2017/2941615
- [33] W. Gao, M.K. Jamil, A Javed, M.R. Farahani, M. Imran. Inverse sum indeg index of the line graphs of subdivision graphs of some chemical structures. UPB Sci. Bulletin B 80 (3), 97-104, 2018.
- [34] S Akhter, M. Imran, W. Gao, M.R. Farahani. On topological indices of honeycomb networks and graphene networks. Hacettepe Journal of Mathematics and Statistics 47 (1), 19-35, 2018.
- [35] X. Zhang, X. Wu, S. Akhter, M.K. Jamil, J.B. Liu, M.R. Farahani. Edge-version atombond connectivity and geometric arithmetic indices of generalized bridge molecular graphs. Symmetry 10 (12), 751, 2018. https://doi.org/10.3390/sym10120751

- [36] H. Yang, A.Q. Baig, W. Khalid, M.R. Farahani, X. Zhang. M-polynomial and topological indices of benzene ring embedded in P-type surface network. Journal of Chemistry 2019, Article ID 7297253, https://doi.org/10.1155/2019/7297253
- [37] D.Y. Shin, S. Hussain, F. Afzal, C. Park, D. Afzal, M.R. Farahani. Closed formulas for some new degree based topological descriptors using Mpolynomial and boron triangular nanotube. Frontiers in Chemistry, 1246, 2021. https://doi.org/10.3389/fchem.2020.613873
- [38] D Afzal, S Ali, F Afzal, M Cancan, S Ediz, M.R. Farahani. A study of newly defined degree-based topological indices via M-polynomial of Jahangir graph. Journal of Discrete Mathematical Sciences and Cryptography 24 (2), 427-438, 2021.