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EXPECTED VALUE FOR THE k-DISTANCE DEGREE INDEX OF A GRAPH

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Abstract. For a graph G, the k-distance degree index is

$$N_k(G) = \sum_{k=1}^{diam(G)} \left(\sum_{w \in V(G)} d_k(w) \right) k.$$

In this article, we calculate the accurate formula of the expected value for k-distance degree index in a random arranged polygonal string with m-arranged polygons. Finally, we determine the average value of this index in the collection of all those arranged polygonal strings.

Mathematics Subject Classification. 05C12, 05C30, 05C80, 05C92, 05D40.

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Introduction

All over this paper, all the graphs are simple, finite and connected. A graph $G = (V, E)$ is with the vertex set V of order $|V| = n$ and the edge set E of size $|E| = m$. For two vertices w and t of G, $d(w, t)$ is the size of the nearest path between them. For vertex $x \in V$ and $k \in \mathbb{Z}$, the open k-neighborhood of x in G, $N_k(x/G)$ or $N_k(x)$, is $N_k(x) = \{y \in V(G) : d(x, y) = k\}$ and the closed k-neighborhood of x in G, $N_k[x/G]$, is $N_k[x/G] = N_k(x/G) \cup \{x\}$. The k-degree of a vertex x in a graph G, $d_k(x/G)$ or $d_k(x)$, is $d_k(x/G) = |N_k(x/G)|$.

A topological index of a graph G is a numerical calculation based on the graph constructions. The topological indices of the chemical structures create relationships among construction of a molecular structure and its chemical properties. There are more topological indices [1–5,14] and several of indices are based on the distance between molecules of a chemical structure. In 1947, the first topological index based on distance is Wiener index [13] defined as

$$W(G) = \sum_{\{w,t\} \in V} d(w, t).$$

In 1993, the Hyper-wiener index was defined by Randic [11] as

$$WW(G) = \frac{1}{2} \sum_{\{w,t\} \in V} (d(w, t) + d^2(w, t)).$$

Keywords. k-distance degree index, expected value, random arranged polygonal string.

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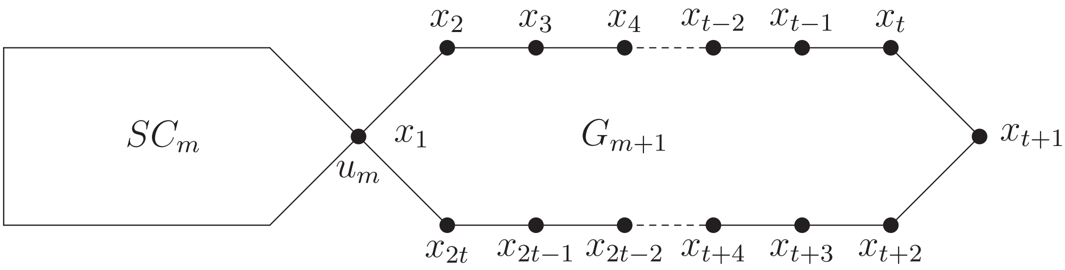

FIGURE 1. A arranged polygonal string SC_{m+1} with $m+1$ arranged polygons.

In 1993, the Harrary index was defined by authors [6, 10] as

$$H(G) = \sum_{\{w,t\} \in V} \frac{1}{d(w,t)}.$$

In 2018, the k-distance degree index or N_k-index was defined by Naji *et al.* [9] as

$$N_k(G) = \sum_{k=1}^{diam(G)} \left(\sum_{x \in V(G)} d_k(x) \right) k.$$

Recently, many authors investigated topological indices of some random polyphenyl string. Liu and Zhan [8] computed expected values for Gutman index and Schultz index in random arranged polygonal strings. In this paper, we compute this value for the k-distance degree index for these random graphs.

The random arranged polygonal string SC_{m+1} with $m+1$ arranged polygons consists of a new arranged polygon G_{m+1} connecting to terminal of a arranged polygonal string SC_m with m arranged polygons, see Figure 1.

Connecting the final arranged polygon G_{m+1} to the front random arranged polygonal string SC_m can do with k methods. They can be defined as $SC^1_{m+1}, SC^2_{m+1}, \cdots, SC^{t-1}_{m+1}$ and SC^t_{m+1} sequentially, see Figure 2.

A random arranged polygonal string SC_m with m arranged polygons could be attained by attaching a arranged polygon at terminal of the string gradual. At every level $r(= 3, 4, \ldots, m)$, a random relation is formed from a state of mentioned in below t probable states:

- $SC_r \to SC^1_{r+1}$ with probability q_1,
- $SC_r \to SC^2_{r+1}$ with probability q_2,

  and so on,
- $SC_r \to SC^{t-1}_{r+1}$ with probability q_{t-1},
- $SC_r \to SC^t_{r+1}$ with probability $q_t = 1 - (\sum_{i=1}^{t-1} q_i)$,

the probabilities $q_1, q_2, \cdots, q_{k-1}$ and q_k are free of the level r.

If $q_1 = 1$ and $q_2 = q_3 = \cdots = q_t = 0$, then meta-string M_m could be attained. If $q_2 = 1$ and $q_1 = q_3 = \cdots = q_t = 0$, then orth-string O^1_m could be attained. If $q_3 = 1$ and $q_1 = q_2 = q_4 = \cdots = q_t = 0$, then orth-string O^2_m could be attained. If $q_{t-1} = 1$ and $q_1 = q_2 = \cdots = q_{t-2} = q_t = 0$, then orth-string O^{t-2}_m could be attained. If $q_t = 1$ and the other $t-1$ probabilities be 0, then para-string P_m could be attained.

THE k-DISTANCE DEGREE INDEX FOR THE RANDOM ARRANGED POLYGONAL STRING

The random arranged polygonal string SC_{m+1}, can be obtained from SC_m by connecting the vertex u_m (u_m is x_1, see Fig. 1) of graph SC_m to a new final arranged polygon G_{m+1}. It is clear that, for every vertex w of

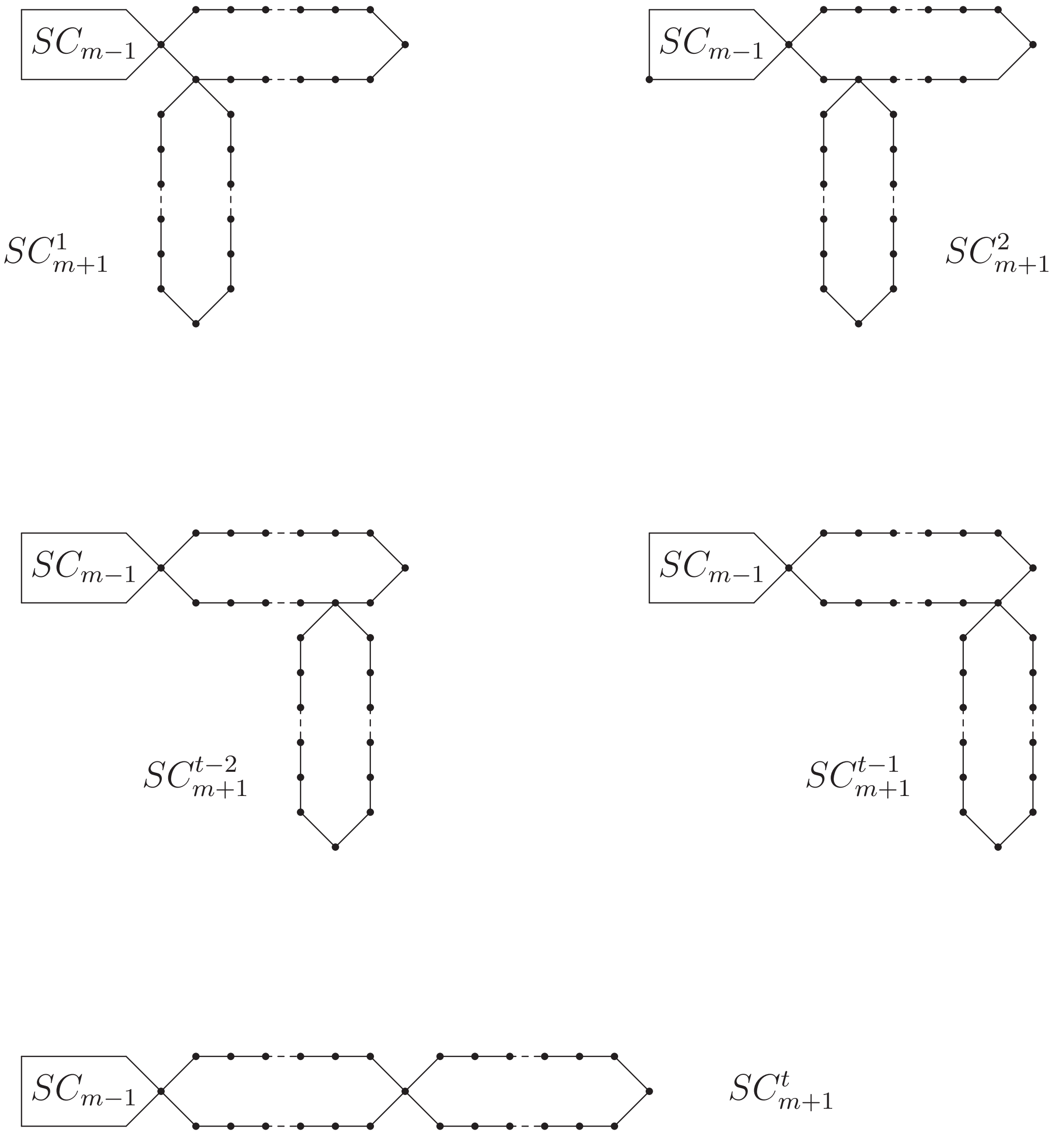

FIGURE 2. The t models of partial regularity of arranged polygonal strings.

SC_m,

$$d(w, x_i) = \begin{cases} d(w, u_m) + i - 1, & 1 \leq i \leq t; \\ d(w, u_m) + 2t + 1 - i, & t + 1 \leq i \leq 2t. \end{cases}$$

Recently, some authors studied the expected values of several indices in random graphs [7, 12]. In this paper, we compute the expected values for k-distance degree index in the random arranged polygonal strings.

Theorem 1. *For $m \geq 1$ and the random graph SC_m, $E(N_k(SC_m))$ is*

$$E(N_k(SC_m)) = \frac{m^3}{3}(2t-1)^2\left(\sum_{i=1}^{t-1}(i-t)q_i + 2t\right) - m^2(2t-1)\left[\left(\sum_{i=1}^{t-1}(i-t)q_i + 2t\right)(2t-2) - t^2\right]$$

$$+ m\left[\left(\sum_{i=1}^{t-1}(i-t)q_i + 2t\right)(2t-1)\left(\frac{4t-11}{3}\right) + 4t^3 + t^2\right]$$
$$+ \left(\sum_{i=1}^{t-1}(i-t)q_i + 2t\right)(4t-2) - 4t^3.$$

Proof. We know that, $N_k(G_{m+1}) = 2t^3$, $|V(SC_m)| = m(2t-1)+1$ and suppose $G = SC_{m+1}$, $Q(i,t) = \sum_{i=1}^{t-1}(i-t)q_i + 2t$.

$$\begin{aligned}
N_k(G) &= N_k(SC_m) + \sum_{w\in SC_m}\left(\sum_{j=2}^{t} 2d(w,x_j) + d(w,x_{t+1})\right) \\
&\quad + N_k(G_{m+1}) + 2\sum_{j=2}^{t}\sum_{w\in SC_m} d(w,x_j) + \sum_{w\in SC_m} d(w,x_{t+1}) \\
&= N_k(SC_m) + N_k(G_{m+1}) + 2\sum_{w\in SC_m}\left(2\sum_{j=2}^{t} d(w,x_j) + d(w,x_{t+1})\right) \\
&= N_k(SC_m) + 2t^3 + 2\sum_{w\in SC_m}\left(2\sum_{j=1}^{t-1}(d(w,u_m)+j) + d(w,u_m) + t\right) \\
&= N_k(SC_m) + 2t^3 + 2\sum_{w\in SC_m}\left((2t-1)d(w,u_m) + t^2\right) \\
&= N_k(SC_m) + 2t^3 + 2(2t-1)\sum_{w\in V(SC_m)} d(w,u_m) + 2t^2[m(2t-1)+1].
\end{aligned}$$

Let we denote the expected value of the random variable $\sum_{w\in V(SC_m)} d(w,u_m)$ by U_m. Hence, we obtain that

$$E(N_k(SC_{m+1})) = E(N_k(SC_m)) + 2(2t-1)U_n + 2t^2(2t-1)m + 2t^2 + 2t^3.$$

According to the following cases, we obtain U_m.

Case 1. $SC_m \to SC_{m+1}^1$, then u_m matches with x_2 or x_{2t}. Therefore, we can represent the $\sum_{w\in V(SC_m)} d(w,u_m)$ by $\sum_{w\in V(SC_m)} d(w,x_2)$ or $\sum_{w\in V(SC_m)} d(w,x_{2t})$ with probability q_1.

Case 2. $SC_m \to SC_{m+1}^2$, then u_m matches with x_3 or x_{2t-1}. Therefore, we can represent the $\sum_{w\in V(SC_m)} d(w,u_m)$ by $\sum_{w\in V(SC_m)} d(w,x_3)$ or $\sum_{w\in V(SC_m)} d(w,x_{2t-1})$ with probability q_2.
And so on,

Case 3. $SC_m \to SC_{m+1}^{t-2}$, then u_m matches with x_{t-1} or x_{t+3}. Therefore, we can represent the $\sum_{w\in V(SC_m)} d(w,u_m)$ by $\sum_{w\in V(SC_m)} d(w,x_{t-1})$ or $\sum_{w\in V(SC_m)} d(w,x_{t+3})$ with probability q_{t-2}.

Case 4. $SC_m \to SC_{m+1}^{t-1}$, then u_m matches with x_t or x_{t+2}. Therefore, we can represent the $\sum_{w\in V(SC_m)} d(w,u_m)$ by $\sum_{w\in V(SC_m)} d(w,x_t)$ or $\sum_{w\in V(SC_m)} d(w,x_{t+2})$ with probability q_{t-1}.

Case 5. $SC_m \to SC_{m+1}^t$, then u_m matches with x_{t+1}. Therefore, we can represent the $\sum_{w\in V(SC_m)} d(w,u_m)$ by $\sum_{w\in V(SC_m)} d(w,x_{t+1})$ with probability $1 - \sum_{i=1}^{t-1} q_i$.

Therefore,

$$U_m = E\left(\sum_{w\in V(SC_m)} d(w,u_m)\right) = q_1\sum_{w\in V(SC_m)} d(w,x_2) + q_2\sum_{w\in V(SC_m)} d(w,x_3) + \cdots$$

$$+ q_{t-1} \sum_{w\in V(SC_m)} d(w,x_t) + \left(1-\sum_{i=1}^{t-1} q_i\right) \sum_{w\in V(SC_m)} d(w,x_{t+1})$$

$$= q_1 \left[\sum_{w\in V(SC_{m-1})} (d(w,u_{m-1})+t+1)\right] + q_2 \left[\sum_{w\in V(SC_{m-1})} (d(w,u_{m-1})+t+2)\right] + \cdots$$

$$+ q_{t-1} \left[\sum_{w\in V(SC_{m-1})} (d(w,u_{m-1})+2t-1)\right] + \left(1-\sum_{i=1}^{t-1} q_i\right) \left[\sum_{w\in V(SC_{m-1})} (d(w,u_{m-1})+2t)\right]$$

$$= U_{m-1} + \left(\sum_{i=1}^{t-1}(i-t)q_i + 2t\right)((m-1)(2t-1)+1)$$

$$= U_{m-1} + Q(i,t)((m-1)(2t-1)+1).$$

In addition, the basic value is $u_1 = \sum_{v\in V(SC_1)} d(v,u_1) = t^2$. Then,

$$U_m = \frac{m^2}{2} Q(i,t)(2t-1) - mQ(i,t)\left(\frac{2t-3}{2}\right) - Q(i,t) + t^2.$$

Therefore,

$$E(N_k(SC_{m+1})) = E(N_k(SC_m)) + 2(2t-1)U_m + 2(2t-1)t^2 m + 2t^2 + 2t^3$$

$$= E(N_k(SC_m)) + 2(2t-1)\left[\frac{m^2}{2} Q(i,t)(2t-1) - mQ(i,t)\left(\frac{2t-3}{2}\right)\right.$$

$$\left. - Q(i,t) + t^2\right] + 2(2t-1)t^2 m + 2t^2 + 2t^3.$$

The basic value is $E(N_k(SC_1)) = 4t(1+2+\cdots+(t-1)) + 2t^2 = 2t^3$. Then,

$$E(N_k(SC_m)) = \frac{m^3}{3}(2t-1)^2 Q(i,t) - m^2(2t-1)[Q(i,t)(2t-2) - t^2]$$

$$+ m\left[Q(i,t)(2t-1)\left(\frac{4t-11}{3}\right) + 4t^3 + t^2\right] + Q(i,t)(4t-2) - 4t^3.$$

Finally, with replacing $Q(i,t) = \sum_{i=1}^{t-1}(i-t)q_i + 2t$,

$$E(N_k(SC_m)) = \frac{m^3}{3}(2t-1)^2 \left(\sum_{i=1}^{t-1}(i-t)q_i + 2t\right) - m^2(2t-1)\left[\left(\sum_{i=1}^{t-1}(i-t)q_i + 2t\right)(2t-2) - t^2\right]$$

$$+ m\left[\left(\sum_{i=1}^{t-1}(i-t)q_i + 2t\right)(2t-1)\left(\frac{4t-11}{3}\right) + 4t^3 + t^2\right]$$

$$+ \left(\sum_{i=1}^{t-1}(i-t)q_i + 2t\right)(4t-2) - 4t^3.$$

□

In accordance with the Theorem 1, we have special models of SC_m as:
If $q_1 = 1$ and $q_j = 0$ for $2 \le j \le t-1$, then $SC_m \cong M_m$.
If $q_2 = 1$ and $q_j = 0$ for $1 \le j \le t-1, j \ne 2$, then $SC_m \cong O^1_m$.

If $q_3 = 1$ and $q_j = 0$ for $1 \leq j \leq t-1, j \neq 3$, then $SC_m \cong O_m^2$ and so on.
If $q_{t-1} = 1$ and $q_j = 0$ for $1 \leq j \leq t-1, j \neq t-1$, then $SC_m \cong O_m^{t-2}$.
If $q_j = 0$ for $1 \leq j \leq t-1$, then $SC_m \cong P_m$.

Theorem 2. *The k-distance degree indices of $M_m, O_m^1, O_m^2, \cdots, O_m^{t-2}$ and P_m are*

$$\begin{aligned}N_k(M_m) &= \frac{m^3}{3}(2t-1)^2(t+1) - m^2(2t-1)[(t+1)(2t-2)-t^2] + m[(t+1)(2t-1) \\ &\quad \times \frac{4t-11}{3} + 4t^3 + t^2] + (t-1)(2-4t^2); \\ N_k(O_m^1) &= \frac{m^3}{3}(2t-1)^2(t+2) - m^2(2t-1)[(t+2)(2t-2)-t^2] + m[(t+2)(2t-1) \\ &\quad \times \frac{4t-11}{3} + 4t^3 + t^2] + (t+2)(4t-2) - 4t^3; \\ N_k(O_m^2) &= \frac{m^3}{3}(2t-1)^2(t+3) - m^2(2t-1)[(t+3)(2t-2)-t^2] + m[(t+3)(2t-1) \\ &\quad \times \frac{4t-11}{3} + 4t^3 + t^2] + (t+3)(4t-2) - 4t^3;\end{aligned}$$

by continuing in the likewise,

$$\begin{aligned}N_k(O_m^{t-2}) &= \frac{m^3}{3}(2t-1)^3 - m^2(2t-1)[(2t-1)(2t-2)-t^2] \\ &\quad + m\left[(2t-1)^2\frac{4t-11}{3} + 4t^3 + t^2\right] + 2(2t-1)^2 - 4t^3; \\ N_k(P_m) &= \frac{m^3}{3}2t(2t-1)^2 - m^2(2t-1)[2t(2t-2)-t^2] \\ &\quad + m\left[2t(2t-1)\frac{4t-11}{3} + 4t^3 + t^2\right] - 4t(t-1)^2.\end{aligned}$$

In accordance with the Theorem 2 and Figure 3, it is clear that for $m \geq 3$

$$N_k(M_m) \leq N_k(O_m^1) \leq N_k(O_m^2) \leq \cdots \leq N_k(O_m^{t-2}) \leq N_k(P_m).$$

Average value of the k-distance degree index

Suppose that $\bar{\eta}_m$ be the collection of all polygonal strings that contains m arranged polygons. In the last part, we calculate the average value of the k-distance degree index of $\bar{\eta}_m$.

$$N_k^{ave}(\bar{\eta}_m) = \frac{1}{|\bar{\eta}_m|}\sum_{G \in G_m} N_k(G).$$

Theorem 3. *The average value of the k-distance degree index about $\bar{\eta}_m$ is*

$$\begin{aligned}N_k^{ave}(\bar{\eta}_m) &= \frac{m^3}{3}(2t-1)^2\left(\frac{3t+1}{2}\right) - m^2(2t-1)\left[\left(\frac{3t+1}{2}\right)(2t-2) - t^2\right] \\ &\quad + m\left[\left(\frac{3t+1}{2}\right)(2t-1)\left(\frac{4t-11}{3}\right) + 4t^3 + t^2\right] + \left(\frac{3t+1}{2}\right)(4t-2) - 4t^3.\end{aligned}$$

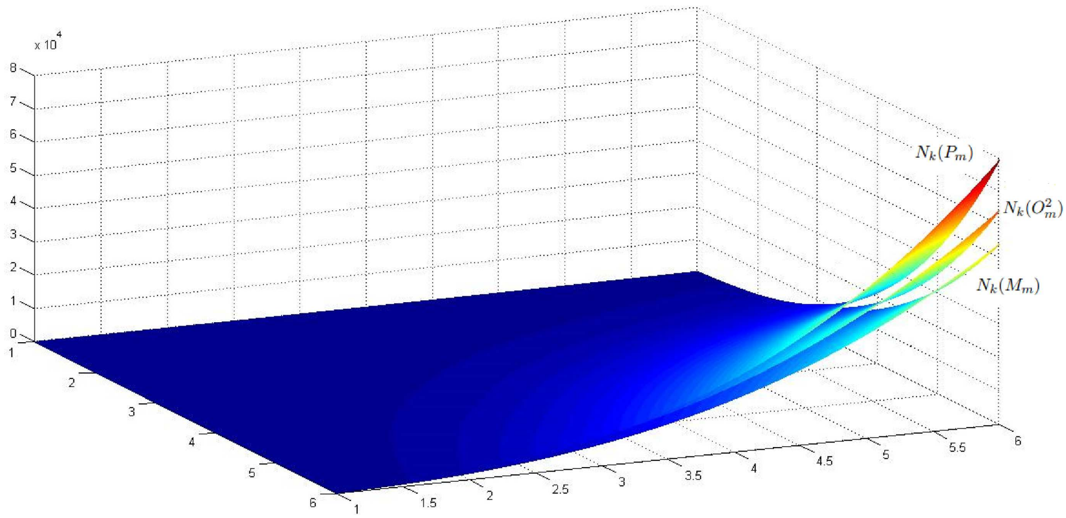

FIGURE 3. Comparison of $N_k(P_m), N_k(O_m^2)$ and $N_k(M_m)$ in arranged polygonal strings.

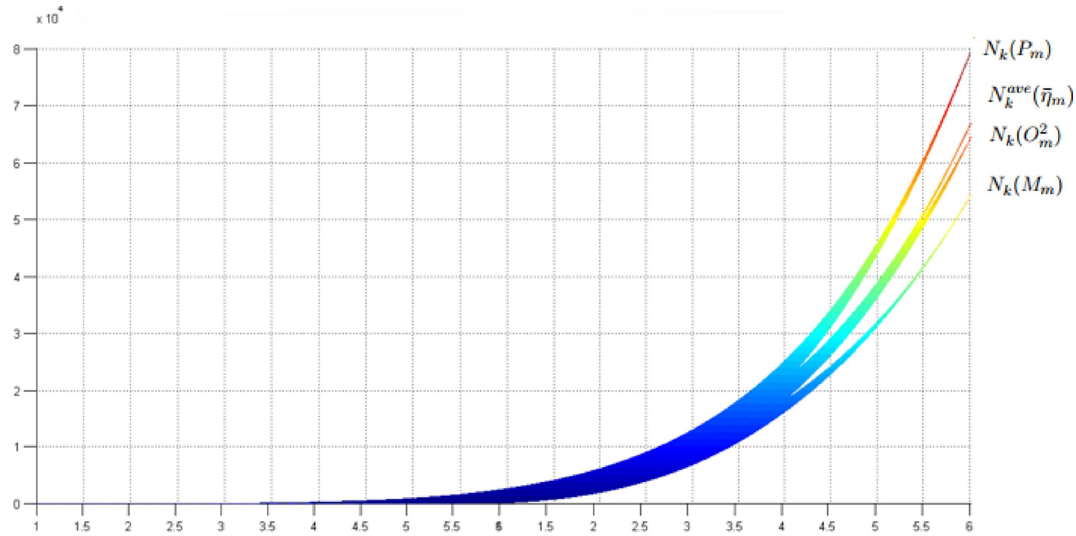

FIGURE 4. Comparison $N_k^{ave}(\bar{\eta}_m)$ with $N_k(P_m), N_k(O_m^2)$ and $N_k(M_m)$ in arranged polygonal strings.

Proof. In Theorem 1, place $q_1 = q_2 = \cdots = q_t = \frac{1}{t}$. □

It is obvious that,

$$N_k^{ave}(\bar{\eta}_m) = \frac{1}{t}\Big[N_k(\bar{M_m}) + N_k(\bar{O_m^1}) + N_k(\bar{O_m^2}) + \cdots + N_k(\bar{O_m^{t-2}}) + N_k(\bar{P_m})\Big].$$

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References

[1] A. Ali and T. Idrees, A note on polyomino chains with extremum general sum-connectivity index. *Commun. Comb. Optim.* **6** (2021) 81–91.

[2] H. Aram and N. Dehgardi, Reformulated F-index of graph operations. *Commun. Comb. Optim.* **2** (2017) 87–98.

[3] M. Ahmad, M. Saeed, M. Javaid and M. Hussain, Exact formula and improved bounds for general sum-connectivity index of graph-operations. *IEEE Access* **7** (2019) 167290–167299.

[4] B. Borovicanin, K.C. Das, B. Furtula and I. Gutman, Bounds for Zagreb indices. *MATCH. Commun. Math. Comput. Chem.* **78** (2017) 17–100.

[5] Z. Du, B. Zhou and N. Trinajstić, On the general sum-connectivity index of trees. *Appl. Math. Lett.* **24** (2011) 402–405.

[6] O. Ivanciuc, T.S. Balaban and A.T. Balaban, Reciprocal distance matrix, related local vertex invariants and topological indices. *J. Math. Chem.* **12** (1993) 309–318.

[7] A.I. Kashkooly, M. Atapour and M. Cancan, The expected values of augmented Zagreb and arithmetic-geometric indices in random polyphenyl chains. *Polycycl. Aromat. Compd.* **43** (2022) 1–12.

[8] X. Liu and Q. Zhan, The expected values for the Gutman index and Schultz index in the random regular polygonal chains. *Molecules* **27** (2022) 6838.

[9] A.M. Naji, S. Nandappa and D.A. Badawi, The k-distance degree index of a graph. *Palest. J. Math.* **2** (2018) 676–687.

[10] D. Plavsic, S. Nikolic, N. Trinajstic and Z. Mihalic, On the Harary index for the characterization of chemical graphs. *J. Math. Chem.* **12** (1993) 235–250.

[11] M. Randic, Novel molecular descriptor for structure–property studies. *Chem. Phys. Lett.* **211** (1993) 478–483.

[12] Z. Raza, The expected values of arithmetic bond connectivity and geometric indices in random phenylene chains. *Heliyon* **6** (2020) 44–79.

[13] H. Wiener, Structural determination of the paraffin boiling points. *J. Am. Chem. Soc.* **69** (1947) 17–20.

[14] B. Zhou and N. Trinajstić, On general sum-connectivity index. *J. Math. Chem.* **47** (2010) 210–218.