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Article

Statistical Analyses of a Class of Random Cyclooctatetraene Chain Networks with Respect to Several Topological Properties [†]

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Abstract: In recent years, there has been a wave of research on complex networks. The purpose of this paper is to study the graph theoretic mathematical properties of random cyclooctatetraene chain. We obtain the explicit analytical expressions for the variances of the Gutman index, Schultz index, multiplicative degree-Kirchhoff index and additive degree-Kirchhoff index of a random cyclooctatetraene chain with n octagons, which plays a crucial role in the research and application of topological indices.

Keywords: random cyclooctatetraene chain; gutman index; schultz index; Multiplicative degree-Kirchhoff index; Additive degree-Kirchhoff index

1. Introduction

In this paper, we only consider simple and finite connected graphs, we refer to [1] and the references cited therein. Chemistry has been widely studied and applied in graph theory. The chemical compounds can be described in chemical graph theory, vertices represent the atoms and edges stand for the covalent bonds between atoms.

The molecular formula of a compound can represent different molecular structures and characteristics, but theoretical chemists are concerned about the physical and chemical properties of a compound and its relationship with the molecular formula of a compound. The topological index is considered as one of the most important methods to establish the relationship between molecular structure and its physicochemical properties in chemical graph theory.

In reality, chemical molecules are various. The same element has different shapes, and the same molecule has different expression names. Hydrocarbons are a kind of very important substances, and their synthesis has always been an important research topic in the field of organic chemistry. Cyclooctatetraene is a typical unsaturated hydrocarbon, so more and more people study its structure and properties, and the research in chemical graph theory is more and more in-depth. In this article, we consider four kinds indices of cyclooctatetraene chains with n octagons. And we simply consider the situation that is Starting from a vertex of a Cyclooctatetraene chain, connecting an edge to another octagon. For more information, we can refer to [16,17,24,29].

Let $G = (V_G, E_G)$ be a graph, whose vertex is set V_G and the edge is set E_G . Then let $d_G(u, v)$ (or $d(u, v)$ for short), which represents the distance between two vertices u and v (of G), that is, u, v - path in G is the shortest path between them. The famous Wiener index (or transmission) $\omega(G)$ of E_G is the sum of distances between all vertex pairs of vertices of G . It was created by H.Wiener in 1947 [34], that is

$$W(G) = \sum_{\{u,v\} \subseteq V_G} d_G(u, v). \quad (1)$$

The Wiener index is one of the best studied, most understood, and widely used molecular shape descriptors, which is based on graph theory. Moreover, it becomes more and more widely used and studied, see [3,8,10,39].

A weighted graph [38] (G, ω) is a graph $G = (V_G, E_G)$ together with the weight function $\omega: V_G \rightarrow \mathbb{N}^+$. Let \oplus denote one of the four arithmetic operations $+$, $-$, \times , \div . Therefore, the weighted Wiener index $W(G, \omega)$ is defined as

$$W(G, \omega) = \frac{1}{2} \sum_{u \in V_G} \sum_{v \in V_G} (\omega(u) \oplus \omega(v)) d_G(u, v). \quad (2)$$

Clearly, if $\omega \equiv 1$ and \oplus represents the operation \times , then $W(G, \omega) = W(G)$.

If \oplus represents the operation \times and $\omega(\cdot) \equiv d_G(\cdot)$, then (2) is equivalent to

$$Gut(G) = \frac{1}{2} \sum_{u \in V_G} \sum_{v \in V_G} (d_G(u) d_G(v)) d_G(u, v) = \sum_{\{u, v\} \subseteq V_G} (d_G(u) d_G(v)) d_G(u, v), \quad (3)$$

It is just the Gutman index. For the study of the possible chemical applications of Gutman index, and similar quantities, as well as their theoretical studies, polycyclic molecules are more difficult cases, see [14].

If \oplus denotes the operation $+$ and $\omega(\cdot) \equiv d_G(\cdot)$, then (2) is equivalent to

$$S(G) = \frac{1}{2} \sum_{u \in V_G} \sum_{v \in V_G} (d_G(u) + d_G(v)) d_G(u, v) = \sum_{\{u, v\} \subseteq V_G} (d_G(u) + d_G(v)) d_G(u, v), \quad (4)$$

And it is just the Schultz index. More articles on developing such a topology indexes of the [6,11,19,35], such as mathematical properties, discrimination and applications refer to [30].

The effective resistance distance $r(x, y)$ is the potential difference between x and y (of G) induced by the unique $x - y$ flow with an intensity of 1 that satisfies Kirchhoffs cycle law [12], for more detailed information in [4,13,20,23]. The Wiener index for non-trees is the Kirchhoff index, this distance function proposed by Klein and Randić [25], defined as

$$Kf(G) = \sum_{\{x, y\} \subseteq V_G} r(x, y), \quad (5)$$

There are introduced the eccentric distance sum and the eccentricity resistance-distance sum, refer to [18,22,26].

The multiplicative degree-Kirchhoff index is proposed by Chen and Zhang in 2007 [7], see [33] to study some details about it, which is defined as

$$Kf^*(G) = \sum_{\{x, y\} \subseteq V_G} d(x) d(y) r(x, y), \quad (6)$$

thus, the invariance of this graph is represented as

$$Kf^*(G) = 2|E_G| \sum_{i=2}^n \frac{1}{\lambda_i}, \quad (7)$$

where $0 = \lambda_1 < \lambda_2 \leq \dots \leq \lambda_n$ are the eigenvalues of $\ell(G)$. Furthermore, $\ell(G)$ is the normalized Laplacian matrix of the graph G , which was proposed by Chung [9]. The normalized Laplacian index and multiplicative degree-Kirchhoff index have important applications in mathematical chemistry and statistics. Their research has attracted more and more researchers' attention.

The additive degree-Kirchhoff index is introduced by Gutman, Feng and Yu in 2012 [15], we refer the papers [32,36], which is defined as

$$Kf^+(G) = \sum_{\{x,y\} \subseteq V_G} (d(x) + d(y))r(x,y). \quad (8)$$

In this paper, we mainly talk about the cyclooctatetraene chain G_n with n octagons, which are constructed by the following way.

Firstly, G_1 is an octagon and G_2 is the Figure 1 graph with 2 octagons.

Secondly, The random cyclooctatetraene chain G_{n+1} with n octagons is constructed by attaching a new terminal octagon H_{n+1} to G_n . We demonstrate this process by Figure 2. As demonstrated in Figure 3, we can attach the terminal hexagon H_{n+1} to G_n in four ways and denote the resulted figures by $G_{n+1}^1, G_{n+1}^2, G_{n+1}^3, G_{n+1}^4$ respectively.

At each step, a random selection is made from one of the following possible constructions:

- $G_n \rightarrow G_{n+1}^1$ with probability p_1 ,
- $G_n \rightarrow G_{n+1}^2$ with probability p_2 ,
- $G_n \rightarrow G_{n+1}^3$ with probability p_3 ,
- $G_n \rightarrow G_{n+1}^4$ with probability $p_4 = 1 - p_1 - p_2 - p_3$,

We consider four random variables $Z_n^1, Z_n^2, Z_n^3, Z_n^4$ as our choice. If our choice is G_{n+1}^i , we let $Z_n^i = 1$, otherwise $Z_n^i = 0$, $i = 1, 2, 3, 4$, we can easily obtain that

$$P(Z_n^i = 1) = p_i, P(Z_n^i = 0) = 1 - p_i, i = 1, 2, 3, 4 \quad (9)$$

and $Z_n^1 + Z_n^2 + Z_n^3 + Z_n^4 = 1$.

By the above processes, we obtain a random polyphenylene chain $G_n(p_1, p_2, p_3, p_4)$. We always abbreviate $G_n(p_1, p_2, p_3, p_4)$ to G_n .

Noting that G_n is a random graph, $Gut(G_n)$, $S(G_n)$, $Kf^*(G_n)$ and $Kf^+(G_n)$ are all random variables in probability. In the view of probability, one problem appears naturally. When n is big enough, whether the distribution of $Gut(G_n)$, $S(G_n)$, $Kf^*(G_n)$ and $Kf^+(G_n)$ will look like a distribution in probability or not.

In this paper, we make the following hypothesis.

Hypothesis 1.1. Our choice of attaching the new terminal hexagon H_{n+1} to G_n , $n = 2, 3, \dots$ are random and independently. In more accurate words, the series of random variables $Z_n^1, Z_n^2, Z_n^3, Z_{n=2}^4$ are independently and have the same law (9). For some $i \in 1, 2, 3$, we have $0 < p_i < 1$. Under Hypothesis 1.1, we give analytical expressions for the variances of $Gut(G_n)$, $S(G_n)$, $Kf^*(G_n)$ and $Kf^+(G_n)$



Figure 1. Graph G_2 .

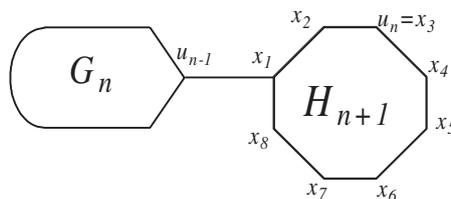


Figure 2. The construction of G_{n+1} from G_n and H_{n+1} .

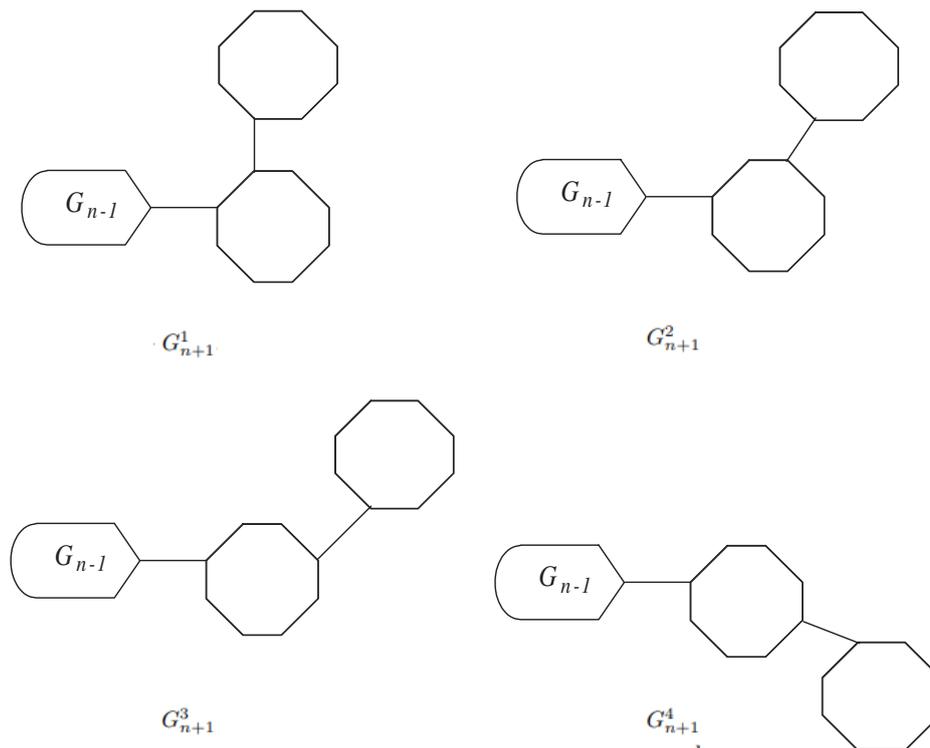


Figure 3. Four ways to attach the new terminal hexagon H_{n+1} to G_n .

2. The variances for the Gutman index and Schultz index of a random cyclooctatetraene chain

For a random cyclooctatetraene chain G_n , the Gutman index and Schultz index are random variables. In this section, we will consider the variances of $Gut(G_n)$ and $S(G_n)$. In fact, G_{n+1} is G_n linked to a new terminal octagon H_{n+1} by an edge, where H_{n+1} is spanned by vertices $x_1, x_2, x_3, x_4, x_5, x_6, x_7, x_8$, and the new edge is $u_n x_1$; see Figure 1. On the hand, for all $v \in V_{G_n}$, one has

$$d(x_1, v) = d(u_n, v) + 1, \quad d(x_2, v) = d(u_n, v) + 2, \quad d(x_3, v) = d(u_n, v) + 3, \quad d(x_4, v) = d(u_n, v) + 4, \quad (10)$$

$$d(x_5, v) = d(u_n, v) + 5, \quad d(x_6, v) = d(u_n, v) + 4, \quad d(x_7, v) = d(u_n, v) + 3, \quad d(x_8, v) = d(u_n, v) + 2, \quad (11)$$

$$\sum_{v \in V_{G_n}} d_{G_{n+1}}(v) = 18n - 1. \quad (12)$$

On the other hand,

$$\sum_{i=1}^8 d(x_i)d(x_1, x_i) = 32, \quad \sum_{i=1}^8 d(x_i)d(x_2, x_i) = 33, \quad \sum_{i=1}^8 d(x_i)d(x_3, x_i) = 34, \quad \sum_{i=1}^8 d(x_i)d(x_4, x_i) = 35, \quad (13)$$

$$\sum_{i=1}^8 d(x_i)d(x_5, x_i) = 36, \quad \sum_{i=1}^8 d(x_i)d(x_6, x_i) = 35, \quad \sum_{i=1}^8 d(x_i)d(x_7, x_i) = 34, \quad \sum_{i=1}^8 d(x_i)d(x_8, x_i) = 33. \quad (14)$$

In [40] Theorem 1, the author proves that

$$E(Gut(G_n)) = (270 - 162p_1 - 108p_2 - 54p_3)n^3 + (486p_1 + 324p_2 + 162p_3 - 90)n^2 + (77 - 324p_1 - 216p_2 - 108p_3)n - 1.$$

Now we introduce the first main result in this section.

Theorem 1. *If Hypothesis 1.1 is true, the following results are obtained. The variance of $Gut(G_n)$, which is the Gutman index of the random cyclooctatetraene chain G_n , is given by*

$$\begin{aligned} \text{Var}(Gut(G_n)) &= \frac{1}{30}(\sigma^2 n^5 - 5rn^4 + 10\tilde{\sigma}^2 n^3 + (65r - 30\sigma^2 - 45\tilde{\sigma}^2)n^2 \\ &\quad + (-120r + 59\sigma^2 + 65\tilde{\sigma}^2)n + (60r - 30\sigma^2 - 30\tilde{\sigma}^2)). \end{aligned}$$

where

$$\begin{aligned} \sigma^2 &= 648^2 p_1 + 972^2 p_2 + 1296^2 p_3 + 1620^2 p_4 - (648p_1 + 972p_2 + 1296p_3 + 1620p_4)^2 \\ \tilde{\sigma}^2 &= 90^2 p_1 + 414^2 p_2 + 738^2 p_3 + 1062^2 p_4 - (90p_1 + 414p_2 + 738p_3 + 1062p_4)^2 \\ r &= 648 \cdot 90 \cdot p_1 + 972 \cdot 414 \cdot p_2 + 1296 \cdot 738 \cdot p_3 + 1620 \cdot 1062 \cdot p_4 \\ &\quad - (648p_1 + 972p_2 + 1296p_3 + 1620p_4) \cdot (90p_1 + 414p_2 + 738p_3 + 1062p_4) \end{aligned}$$

Proof. Let

$$A_n := 18 \sum_{v \in V_{G_n}} d(v)d(u_n, v).$$

then, by [40] (5.1), we obtain

$$Gut(G_{n+1}) = Gut(G_n) + A_n + 882n + 239. \quad (15)$$

Recalling that $Z_n^1, Z_n^2, Z_n^3, Z_n^4$ are random variables in Section 1 which indicate our choice in the construction of G_{n+1} from G_n . We have the following four equalities.

Equality 1.

$$A_n Z_n^1 = (A_{n-1} + 648n - 90)Z_n^1$$

If $Z_n^1 = 0$, the above equality is obvious. So we only need to consider the case $Z_n^1 = 1$, which implies $G_n \rightarrow G_{n+1}^1$. In this case, u_n (of G_n) coincides with the vertex labelled x_2 or x_8 (of H_n), see Figure 4. In this situation, A_n becomes

$$\begin{aligned} 18 \sum_{v \in V_{G_n}} d(v)d(x_2, v) &= 18 \sum_{v \in V_{G_{n-1}}} d(v)d(x_2, v) + 18 \sum_{v \in V_{H_n}} d(v)d(x_2, v) \\ &= 18 \sum_{v \in V_{G_{n-1}}} d(v)(d(v, u_{n-1}) + d(x_2, u_{n-1})) + 18 \times 33 \\ &= 18 \sum_{v \in V_{G_{n-1}}} d(v)(d(v, u_{n-1}) + 2) + 18 \times 33 \\ &= A_{n-1} + 36 \sum_{v \in V_{G_{n-1}}} d(v) + 594 \\ &= A_{n-1} + 36(18n - 19) + 594 \\ &= A_{n-1} + 648n - 90, \end{aligned}$$

in the above, we have used (10)-(12). Thus, we conclude the desired equality.

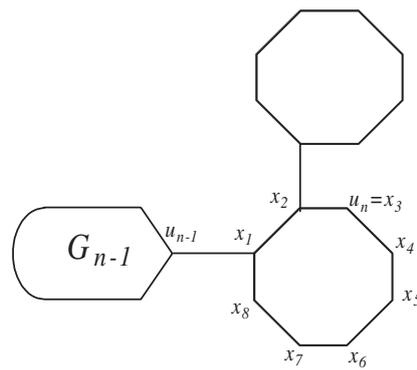


Figure 4. $G_n \rightarrow G_{n+1}^1$.

Equality 2.

$$A_n Z_n^2 = (A_{n-1} + 972n - 414) Z_n^2$$

As that in the proof of Equality 1, we only consider the case $Z_n^2 = 1$, that is $G_n \rightarrow G_{n+1}^2$. The proof is similar and we omit the details.

Equality 3.

$$A_n Z_n^3 = (A_{n-1} + 1296n - 738) Z_n^3$$

we only consider the case $Z_n^3 = 1$, that is $G_n \rightarrow G_{n+1}^3$. The proof is the same as Equality 1 and we omit the details.

Equality 4.

$$A_n Z_n^4 = (A_{n-1} + 1620n - 1062) Z_n^4$$

we only consider the case $Z_n^4 = 1$, that is $G_n \rightarrow G_{n+1}^4$. The proof is also similar and we omit the details.

Noting that $Z_n^1 + Z_n^2 + Z_n^3 + Z_n^4 = 1$, by the above discussions, it holds that

$$\begin{aligned} A_n &= A_n(Z_n^1 + Z_n^2 + Z_n^3 + Z_n^4) \\ &= (A_{n-1} + 648n - 90)Z_n^1 + (A_{n-1} + 972n - 414)Z_n^2 + (A_{n-1} + 1296n - 738)Z_n^3 + (A_{n-1} + 1620n - 1062)Z_n^4 \\ &= A_{n-1} + (648Z_n^1 + 972Z_n^2 + 1296Z_n^3 + 1620Z_n^4)n - (90Z_n^1 + 414Z_n^2 + 738Z_n^3 + 1062Z_n^4) \\ &= A_{n-1} + nU_n - V_n \end{aligned}$$

where for each n ,

$$U_n = 648Z_n^1 + 972Z_n^2 + 1296Z_n^3 + 1620Z_n^4, V_n = 90Z_n^1 + 414Z_n^2 + 738Z_n^3 + 1062Z_n^4.$$

Therefore, by (15) we obtain

$$\begin{aligned}
Gut(G_n) &= Gut(G_1) + \sum_{i=1}^{n-1} A_i + \sum_{i=1}^{n-1} (882i + 239) \\
&= Gut(G_1) + \sum_{i=1}^{n-1} \left(\sum_{j=1}^{i-1} (A_{j+1} - A_j) + A_1 \right) + \sum_{i=1}^{n-1} (882i + 239) \\
&= Gut(G_1) + \sum_{i=1}^{n-1} \sum_{j=1}^{i-1} (A_{j+1} - A_j) + (n-1)A_1 + \sum_{i=1}^{n-1} (882i + 239) \\
&= Gut(G_1) + \sum_{i=1}^{n-1} \sum_{j=1}^{i-1} ((j+1)U_{j+1} - V_{j+1}) + (n-1)A_1 + \sum_{i=1}^{n-1} (882i + 239) \\
&= Gut(G_1) + \sum_{i=1}^{n-1} \sum_{j=1}^{i-1} ((j+1)U_{j+1} - V_{j+1}) + O(n^2)
\end{aligned}$$

By direct calculation, one sees that $Var(U_j) = \sigma^2$, $Var(V_j) = \tilde{\sigma}^2$, $Cov(U_j, V_j) = r$, where for any two random variables X, Y , $Cov(X, Y) := E(XY) - E(X)E(Y)$. By the properties of variance and interchanging the order of sums, it follows that

$$\begin{aligned}
Var(Gut(G_n)) &= Var\left(\sum_{i=1}^{n-1} \sum_{j=1}^{i-1} ((j+1)U_{j+1} - V_{j+1})\right) \\
&= Var\left(\sum_{j=1}^{n-2} \sum_{i=j+1}^{n-1} ((j+1)U_{j+1} - V_{j+1})\right) \\
&= Var\left(\sum_{j=1}^{n-2} ((j+1)U_{j+1} - V_{j+1})(n-j-1)\right) \\
&= \sum_{j=1}^{n-2} (n-j-1)^2 Var((j+1)U_{j+1} - V_{j+1}) \\
&= \sum_{j=1}^{n-2} (n-j-1)^2 Cov((j+1)U_{j+1} - V_{j+1}, (j+1)U_{j+1} - V_{j+1}) \\
&= \sum_{j=1}^{n-2} (n-j-1)^2 ((j+1)^2 Cov(U_{j+1}, U_{j+1}) - 2(j+1)Cov(U_{j+1}, V_{j+1}) + Cov(V_{j+1}, V_{j+1})) \\
&= \sum_{j=1}^{n-2} (n-j-1)^2 ((j+1)^2 \sigma^2 - 2(j+1)r + \tilde{\sigma}^2)
\end{aligned}$$

With the help of a computer, the above equality implies the desired result $Var(Gut(G_n))$.

Now, we discuss the variance of the Schultz index of a random cyclooctatetraene chain.

In [40] Theorem 2.3, we have

$$\begin{aligned}
E(S(G_n)) &= (240 - 144p_1 - 96p_2 - 48p_3)n^3 + (432p_1 + 288p_2 + 144p_3 - 40)n^2 \\
&\quad + (56 - 288p_1 - 192p_2 - 96p_3)n.
\end{aligned}$$

Then we state our results.

Theorem 2. Assume Hypothesis 1.1, then the following results hold. The variance of $S(G_n)$, which is the Schultz index of the random cyclooctatetraene G_n , is given by

$$\begin{aligned}
Var(S(G_n)) &= \frac{1}{30} (\sigma^2 n^5 - 5rn^4 + 10\tilde{\sigma}^2 n^3 + (65r - 30\sigma^2 - 45\tilde{\sigma}^2)n^2 \\
&\quad + (-120r + 59\sigma^2 + 65\tilde{\sigma}^2)n + (60r - 30\sigma^2 - 30\tilde{\sigma}^2)).
\end{aligned}$$

where

$$\begin{aligned}\sigma^2 &= 576^2 p_1 + 864^2 p_2 + 1152^2 p_3 + 1440^2 p_4 - (576 p_1 + 864 p_2 + 1152 p_3 + 1440 p_4)^2 \\ \tilde{\sigma}^2 &= 40^2 p_1 + 328^2 p_2 + 616^2 p_3 + 904^2 p_4 - (40 p_1 + 328 p_2 + 616 p_3 + 904 p_4)^2 \\ r &= 576 \cdot 40 \cdot p_1 + 864 \cdot 328 \cdot p_2 + 1152 \cdot 616 \cdot p_3 + 1440 \cdot 904 \cdot p_4 \\ &\quad - (576 p_1 + 864 p_2 + 1152 p_3 + 1440 p_4) \cdot (40 p_1 + 328 p_2 + 616 p_3 + 904 p_4)\end{aligned}$$

Proof. by [40] (5.2), we obtain

$$S(G_{n+1}) = S(G_n) + 18 \sum_{v \in V_{G_n}} d(u_n, v) + 8 \sum_{v \in V_{G_n}} d(v) d(u_n, v) + 824n + 248. \quad (16)$$

where

$$B_n := \sum_{v \in V_{G_n}} (18 + 8d(v)) d(u_n, v).$$

$$S(G_{n+1}) = S(G_n) + B_n + 824n + 248.$$

With similar discussion, we have the following four equalities.

Equality 1.

$$B_n Z_n^1 = (B_{n-1} + 576n - 40) Z_n^1$$

If $Z_n^1 = 0$, the above equality is obvious. So we only need to consider the case $Z_n^1 = 1$, which implies $G_n \rightarrow G_{n+1}^1$. In this case, u_n (of G_n) coincides with the vertex labelled x_2 or x_8 (of H_n), see Figure 4. In this situation, B_n becomes

$$\begin{aligned}B_n &= \sum_{v \in V_{G_n}} (18 + 8d(v)) d(x_2, v) \\ &= \sum_{v \in V_{G_{n-1}}} (18 + 8d(v)) d(x_2, v) + \sum_{v \in V_{H_n}} (18 + 8d(v)) d(x_2, v) \\ &= \sum_{v \in V_{G_{n-1}}} (18 + 8d(v)) (d(u_{n-1}, v) + 2) + 18 \times 16 + 8 \times 33 \\ &= \sum_{v \in V_{G_{n-1}}} (18 + 8d(v)) d(u_{n-1}, v) + 2 \sum_{v \in V_{G_{n-1}}} (18 + 8d(v)) + 18 \times 16 + 8 \times 33 \\ &= \sum_{v \in V_{G_{n-1}}} (18 + 8d(v)) d(u_{n-1}, v) + 2(18 \times 8(n-1) + 8 \times (18(n-1) - 1)) + 18 \times 16 + 8 \times 33 \\ &= B_{n-1} + 2(288n - 296) + 552 \\ &= B_{n-1} + 576n - 40\end{aligned}$$

in the above, we have used (10)-(12). Thus, we conclude the desired equality.

Equality 2.

$$B_n Z_n^2 = (B_{n-1} + 864n - 328) Z_n^2$$

As that in the proof of Equality 1, we only consider the case $Z_n^2 = 1$, that is $G_n \rightarrow G_{n+1}^2$. The proof is similar and we omit the details.

Equality 3.

$$B_n Z_n^3 = (B_{n-1} + 1152n - 616) Z_n^3$$

we only consider the case $Z_n^3 = 1$, that is $G_n \longrightarrow G_{n+1}^3$. The proof is the same as Equality 1 and we omit the details.

Equality 4.

$$B_n Z_n^4 = (B_{n-1} + 1440n - 904) Z_n^4$$

we only consider the case $Z_n^4 = 1$, that is $G_n \longrightarrow G_{n+1}^4$. The proof is also similar and we omit the details.

Noting that $Z_n^1 + Z_n^2 + Z_n^3 + Z_n^4 = 1$, by the above discussions, it holds that

$$\begin{aligned} B_n &= B_n(Z_n^1 + Z_n^2 + Z_n^3 + Z_n^4) \\ &= B_{n-1} + nU_n - V_n \end{aligned}$$

where for each n ,

$$U_n = 576Z_n^1 + 864Z_n^2 + 1152Z_n^3 + 1440Z_n^4, V_n = 40Z_n^1 + 328Z_n^2 + 616Z_n^3 + 904Z_n^4.$$

Therefore, by (15)

$$\begin{aligned} S(G_n) &= S(G_1) + \sum_{i=1}^{n-1} B_i + \sum_{i=1}^{n-1} (824i + 248) \\ &= S(G_1) + \sum_{i=1}^{n-1} \left(\sum_{j=1}^{i-1} (B_{j+1} - B_j) + B_1 \right) + \sum_{i=1}^{n-1} (824i + 248) \\ &= S(G_1) + \sum_{i=1}^{n-1} \sum_{j=1}^{i-1} (B_{j+1} - B_j) + (n-1)B_1 + \sum_{i=1}^{n-1} (824i + 248) \\ &= S(G_1) + \sum_{i=1}^{n-1} \sum_{j=1}^{i-1} ((j+1)U_{j+1} - V_{j+1}) + (n-1)B_1 + \sum_{i=1}^{n-1} (824i + 248) \\ &= S(G_1) + \sum_{i=1}^{n-1} \sum_{j=1}^{i-1} ((j+1)U_{j+1} - V_{j+1}) + O(n^2) \end{aligned}$$

If we replace $Gut(G_n)$ by $S(G_n)$ in the proof of Theorem 1, the rest proof of this theorem is the same as that in the proof of Theorem 1 and we omit the details.

3. The variances of multiplicative and additive degree-Kirchhoff indices of a random cyclooctatetraene chain

In this section, we talk about the variances for $Kf^*(G_n)$ and $Kf^+(G_n)$. For a random cyclooctatetraene chain G_n , the multiplicative degree-Kirchhoff index $Kf^*(G_n)$ and the additive degree-Kirchhoff index $Kf^+(G_n)$ are random variables.

Recall that G_{n+1} is obtained by attaching G_n a new terminal octagon H_{n+1} by an edge, where H_{n+1} is spanned by vertices $x_1, x_2, x_3, x_4, x_5, x_6, x_7, x_8$, and the new edge is $u_n x_1$; see Figure 1. On the hand, for all $v \in V_{G_n}$, one has

$$r(x_1, v) = r(u_n, v) + 1, r(x_2, v) = r(u_n, v) + 1 + \frac{7}{8}, r(x_3, v) = r(u_n, v) + 1 + \frac{12}{8}, r(x_4, v) = r(u_n, v) + 1 + \frac{15}{8}, \quad (17)$$

$$r(x_5, v) = r(u_n, v) + 1 + \frac{16}{8}, r(x_6, v) = r(u_n, v) + 1 + \frac{15}{8}, r(x_7, v) = r(u_n, v) + 1 + \frac{12}{8}, r(x_8, v) = r(u_n, v) + 1 + \frac{7}{8}. \quad (18)$$

$$\sum_{v \in V_{G_n}} d_{G_{n+1}}(v) = 18n - 1. \quad (19)$$

On the other hand,

$$\sum_{i=1}^8 d(x_i)r(x_1, x_i) = 21, \sum_{i=1}^8 d(x_i)r(x_2, x_i) = \frac{175}{8}, \sum_{i=1}^8 d(x_i)r(x_3, x_i) = \frac{45}{2}, \sum_{i=1}^8 d(x_i)r(x_4, x_i) = \frac{183}{8}, \quad (20)$$

$$\sum_{i=1}^8 d(x_i)r(x_5, x_i) = 23, \sum_{i=1}^8 d(x_i)r(x_6, x_i) = \frac{183}{8}, \sum_{i=1}^8 d(x_i)r(x_7, x_i) = \frac{45}{2}, \sum_{i=1}^8 d(x_i)r(x_8, x_i) = \frac{175}{8}. \quad (21)$$

In [40] Theorem 3, we have

$$\begin{aligned} E(Kf^*(G_n)) &= (162 - \frac{243}{4}p_1 - 27p_2 - \frac{27}{4}p_3)n^3 + (36 + \frac{729}{4}p_1 + 81p_2 + \frac{81}{4}p_3)n^2 \\ &\quad - (29 + \frac{243}{2}p_1 + 54p_2 + \frac{27}{2}p_3)n - 1. \end{aligned}$$

Now we introduce the first main result in this section.

Theorem 3. Assume Hypothesis 1.1, then the following results hold. The variance of $Kf^*(G_n)$, which is the multiplicative degree-Kirchhoff index of the random cyclooctatetraene G_n , is given by

$$\begin{aligned} \text{Var}(Kf^*(G_n)) &= \frac{1}{30}(\sigma^2 n^5 - 5rn^4 + 10\tilde{\sigma}^2 n^3 + (65r - 30\sigma^2 - 45\tilde{\sigma}^2)n^2 \\ &\quad + (-120r + 59\sigma^2 + 65\tilde{\sigma}^2)n + (60r - 30\sigma^2 - 30\tilde{\sigma}^2)). \end{aligned}$$

where

$$\begin{aligned} \sigma^2 &= (\frac{1215}{2})^2 p_1 + 810^2 p_2 + (\frac{1863}{2})^2 p_3 + 972^2 p_4 - (\frac{1215}{2}p_1 + 810p_2 + \frac{1863}{2}p_3 + 972p_4)^2 \\ \tilde{\sigma}^2 &= (\frac{495}{2})^2 p_1 + 450^2 p_2 + (\frac{1143}{2})^2 p_3 + 612^2 p_4 - (\frac{495}{2}p_1 + 450p_2 + \frac{1143}{2}p_3 + 612p_4)^2 \\ r &= \frac{1215}{2} \cdot \frac{495}{2} \cdot p_1 + 810 \cdot 450 \cdot p_2 + \frac{1863}{2} \cdot \frac{1143}{2} \cdot p_3 + 972 \cdot 612 \cdot p_4 \\ &\quad - (\frac{1215}{2}p_1 + 810p_2 + \frac{1863}{2}p_3 + 972p_4) \cdot (\frac{495}{2}p_1 + 450p_2 + \frac{1143}{2}p_3 + 612p_4) \end{aligned}$$

Proof. by [40] (5.3), we see

$$Kf^*(G_{n+1}) = Kf^*(G_n) + 18 \sum_{v \in V_{G_n}} d(v)r(u_n, v) + 684n + 151. \quad (22)$$

where

$$C_n := 18 \sum_{v \in V_{G_n}} d(v)r(u_n, v). \quad (23)$$

$$Kf^*(G_{n+1}) = Kf^*(G_n) + C_n + 684n + 151. \quad (24)$$

Recalling that $Z_n^1, Z_n^2, Z_n^3, Z_n^4$ are random variables in Section 1 which indicate our choice in the construction of G_{n+1} from G_n . We have the following four equalities.

Equality 1.

$$C_n Z_n^1 = (C_{n-1} + \frac{1215}{2}n - \frac{495}{2})Z_n^1$$

If $Z_n^1 = 0$, the above equality is obvious. So we only need to consider the case $Z_n^1 = 1$, which implies $G_n \rightarrow G_{n+1}^1$. In this case, u_n (of G_n) coincides with the vertex labelled x_2 or x_8 (of H_n), see Fig. 4. In this situation, C_n becomes

$$\begin{aligned} C_n &= 18 \sum_{v \in V_{G_n}} d(v)r(x_2, v) \\ &= 18 \sum_{v \in V_{G_{n-1}}} d(v)r(x_2, v) + 18 \sum_{v \in V_{H_n}} d(v)r(x_2, v) \\ &= 18 \sum_{v \in V_{G_{n-1}}} d(v)(1 + \frac{7}{8} + r(u_{n-1}, v)) + \frac{175}{8} \times 18 \\ &= 18 \sum_{v \in V_{G_{n-1}}} d(v)r(u_{n-1}, v) + \frac{270}{8} \sum_{v \in V_{G_{n-1}}} d(v) + \frac{175}{8} \times 18 \\ &= C_{n-1} + \frac{270}{8}(18n - 19) + \frac{3150}{8} \\ &= C_{n-1} + \frac{1215}{2}n - \frac{495}{2} \end{aligned}$$

in the above, we have used (17)-(19). Thus, we conclude the desired equality.

Equality 2.

$$C_n Z_n^2 = (C_{n-1} + 810n - 450)Z_n^2$$

As that in the proof of Equality 1, we only consider the case $Z_n^2 = 1$, that is $G_n \rightarrow G_{n+1}^2$. The proof is similar and we omit the details.

Equality 3.

$$C_n Z_n^3 = (C_{n-1} + \frac{1863}{2}n - \frac{1143}{2})Z_n^3$$

we only consider the case $Z_n^3 = 1$, that is $G_n \rightarrow G_{n+1}^3$. The proof is the same as Equality 1 and we omit the details.

Equality 4.

$$C_n Z_n^4 = (C_{n-1} + 972n - 612)Z_n^4$$

we only consider the case $Z_n^4 = 1$, that is $G_n \rightarrow G_{n+1}^4$. The proof is also similar and we omit the details.

Noting that $Z_n^1 + Z_n^2 + Z_n^3 + Z_n^4 = 1$, by the above discussions, it holds that

$$\begin{aligned} C_n &= C_n(Z_n^1 + Z_n^2 + Z_n^3 + Z_n^4) \\ &= C_{n-1} + nU_n - V_n \end{aligned}$$

where for each n ,

$$U_n = \frac{1215}{2}Z_n^1 + 810Z_n^2 + \frac{1863}{2}Z_n^3 + 972Z_n^4, V_n = \frac{495}{2}Z_n^1 + 450Z_n^2 + \frac{1143}{2}Z_n^3 + 612Z_n^4.$$

Therefore, by (22)

$$\begin{aligned} Kf^*(G_n) &= Kf^*(G_1) + \sum_{i=1}^{n-1} C_i + \sum_{i=1}^{n-1} (684i + 151) \\ &= Kf^*(G_1) + \sum_{i=1}^{n-1} \left(\sum_{j=1}^{i-1} (C_{j+1} - C_j) + C_1 \right) + \sum_{i=1}^{n-1} (684i + 151) \\ &= Kf^*(G_1) + \sum_{i=1}^{n-1} \sum_{j=1}^{i-1} (C_{j+1} - C_j) + (n-1)C_1 + \sum_{i=1}^{n-1} (684i + 151) \\ &= Kf^*(G_1) + \sum_{i=1}^{n-1} \sum_{j=1}^{i-1} ((j+1)U_{j+1} - V_{j+1}) + (n-1)C_1 + \sum_{i=1}^{n-1} (684i + 151) \\ &= Kf^*(G_1) + \sum_{i=1}^{n-1} \sum_{j=1}^{i-1} ((j+1)U_{j+1} - V_{j+1}) + O(n^2) \end{aligned}$$

Now we consider $Kf^+(G_n)$, in [40] Theorem 3.3, we have

$$\begin{aligned} E(Kf^+(G_n)) &= (144 - 54p_1 - 24p_2 - 6p_3)n^3 + (61 + 162p_1 + 72p_2 + 18p_3)n^2 \\ &\quad - (37 + 108p_1 + 48p_2 + 12p_3)n. \end{aligned}$$

The variance of $Kf^+(G_n)$, is given by

Theorem 4.

$$\begin{aligned} \text{Var}(Kf^+(G_n)) &= \frac{1}{30}(\sigma^2 n^5 - 5rn^4 + 10\tilde{\sigma}^2 n^3 + (65r - 30\sigma^2 - 45\tilde{\sigma}^2)n^2 \\ &\quad + (-120r + 59\sigma^2 + 65\tilde{\sigma}^2)n + (60r - 30\sigma^2 - 30\tilde{\sigma}^2)). \end{aligned}$$

where

$$\begin{aligned} \sigma^2 &= 540^2 p_1 + 720^2 p_2 + 828^2 p_3 + 864^2 p_4 - (540p_1 + 720p_2 + 828p_3 + 864p_4)^2 \\ \tilde{\sigma}^2 &= 191^2 p_1 + 371^2 p_2 + 479^2 p_3 + 515^2 p_4 - (191p_1 + 371p_2 + 479p_3 + 515p_4)^2 \\ r &= 540 \cdot 191 \cdot p_1 + 720 \cdot 371 \cdot p_2 + 828 \cdot 479 \cdot p_3 + 864 \cdot 515 \cdot p_4 \\ &\quad - (540p_1 + 720p_2 + 828p_3 + 864p_4) \cdot (191p_1 + 371p_2 + 479p_3 + 515p_4) \end{aligned}$$

Proof. by [40] (5.4), we see that

$$Kf^+(G_{n+1}) = Kf^+(G_n) + 18 \sum_{v \in V_{G_n}} r(u_n, v) + 8 \sum_{v \in V_{G_n}} d(v)r(u_n, v) + 637n + 160. \quad (25)$$

where

$$D_n := \sum_{v \in V_{G_n}} (18 + 8d(v))r(u_n, v). \quad (26)$$

$$Kf^+(G_{n+1}) = Kf^+(G_n) + D_n + 637n + 160. \quad (27)$$

Recalling that $Z_n^1, Z_n^2, Z_n^3, Z_n^4$ are random variables in Section 1 which indicate our choice in the construction of G_{n+1} from G_n . We have the following four equalities.

Equality 1.

$$D_n Z_n^1 = (D_{n-1} + 540n - 191)Z_n^1$$

If $Z_n^1 = 0$, the above equality is obvious. So we only need to consider the case $Z_n^1 = 1$, which implies $G_n \rightarrow G_{n+1}^1$. In this case, u_n (of G_n) coincides with the vertex labelled x_2 or x_8 (of H_n), see Figure 4. In this situation, D_n becomes

$$\begin{aligned} \sum_{v \in V_{G_n}} (18 + 8d(v))r(x_2, v) &= 18 \sum_{v \in V_{G_n}} d(v)r(x_2, v) \\ &= \sum_{v \in V_{G_{n-1}}} (18 + 8d(v))r(x_2, v) + \sum_{v \in V_{H_n}} (18 + 8d(v))r(x_2, v) \\ &= \sum_{v \in V_{G_{n-1}}} (18 + 8d(v))(r(u_{n-1}, v) + 1 + \frac{7}{8}) + 18 \sum_{v \in V_{H_n}} r(x_2, x_i) + 8 \sum_{v \in V_{H_n}} d(x_i)r(x_2, x_i) \\ &= \sum_{v \in V_{G_{n-1}}} (18 + 8d(v))r(u_{n-1}, v) + \frac{15}{8} \sum_{v \in V_{G_{n-1}}} (18 + 8d(v)) + 18 \times \frac{14 + 24 + 30 + 16}{8} + 8 \times \frac{175}{8} \\ &= D_{n-1} + \frac{15}{8}(288n - 296) + 364 \\ &= D_{n-1} + 540n - 191 \end{aligned}$$

in the above, we have used (17)-(19). Thus, we conclude the desired equality.

Equality 2.

$$D_n Z_n^2 = (D_{n-1} + 720n - 371)Z_n^2$$

As that in the proof of Equality 1, we only consider the case $Z_n^2 = 1$, that is $G_n \rightarrow G_{n+1}^2$. The proof is similar and we omit the details.

Equality 3.

$$D_n Z_n^3 = (D_{n-1} + 828n - 479)Z_n^3$$

we only consider the case $Z_n^3 = 1$, that is $G_n \rightarrow G_{n+1}^3$. The proof is the same as Equality 1 and we omit the details.

Equality 4.

$$D_n Z_n^4 = (D_{n-1} + 864n - 515)Z_n^4$$

we only consider the case $Z_n^4 = 1$, that is $G_n \rightarrow G_{n+1}^4$. The proof is also similar and we omit the details.

Noting that $Z_n^1 + Z_n^2 + Z_n^3 + Z_n^4 = 1$, by the above discussions, it holds that

$$\begin{aligned} D_n &= D_n(Z_n^1 + Z_n^2 + Z_n^3 + Z_n^4) \\ &= D_{n-1} + nU_n - V_n \end{aligned}$$

where for each n ,

$$U_n = 540Z_n^1 + 720Z_n^2 + 828Z_n^3 + 864Z_n^4, V_n = 191Z_n^1 + 371Z_n^2 + 479Z_n^3 + 515Z_n^4.$$

Therefore, by (25)

$$\begin{aligned}
Kf^+(G_n) &= Kf^+(G_1) + \sum_{i=1}^{n-1} D_i + \sum_{i=1}^{n-1} (637i + 160) \\
&= Kf^+(G_1) + \sum_{i=1}^{n-1} \left(\sum_{j=1}^{i-1} (D_{j+1} - D_j) + D_1 \right) + \sum_{i=1}^{n-1} (637i + 160) \\
&= Kf^+(G_1) + \sum_{i=1}^{n-1} \sum_{j=1}^{i-1} (D_{j+1} - D_j) + (n-1)D_1 + \sum_{i=1}^{n-1} (637i + 160) \\
&= Kf^+(G_1) + \sum_{i=1}^{n-1} \sum_{j=1}^{i-1} ((j+1)U_{j+1} - V_{j+1}) + (n-1)D_1 + \sum_{i=1}^{n-1} (637i + 160) \\
&= Kf^+(G_1) + \sum_{i=1}^{n-1} \sum_{j=1}^{i-1} ((j+1)U_{j+1} - V_{j+1}) + O(n^2)
\end{aligned}$$

If we replace $Gut(G_n)$ by $Kf^+(G_n)$ in the proof of Theorem 1, the rest proof of this theorem is the same as that in the proof of Theorem 1, we simply omit the details.

4. Concluding remarks

In this paper, we obtain the explicit analytical expressions for the variances of the Gutman index, Schultz index, multiplicative degree-Kirchhoff index and additive degree-Kirchhoff index of a random cyclooctatetraene chain with n octagons. All these results will contribute to the study of the Gutman index, Schultz index, multiplicative degree-Kirchhoff index and additive degree-Kirchhoff index of graphs.

With the continuous development and progress of science, more and more molecules are discovered and created. In chemical graph theory, the matter of polygonal chain is being widely studied by researchers. The molecular structures of polygonal chemicals are various and its physicochemical properties also become more and more important which are referenced to [2,5,27,31]. It is possible to establish exact formulas for the variances of some indices of a random polygon chain with n regular polygons.

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