

The Ratio and Product of the Multiplicative Zagreb Indices

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ABSTRACT

The first multiplicative Zagreb index $\Pi_1(G)$ is equal to the product of squares of the degree of the vertices and the second multiplicative Zagreb index $\Pi_2(G)$ is equal to the product of the products of the degree of pairs of adjacent vertices of the underlying molecular graphs G . Also, the multiplicative sum Zagreb index $\Pi_3(G)$ is equal to the product of the sums of the degree of pairs of adjacent vertices of G . In this paper, we introduce a new version of the multiplicative sum Zagreb index and study the moments of the ratio and product of all indices in a randomly chosen molecular graph with tree structure of order n . Also, a supermartingale is introduced by Doob's supermartingale inequality.

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1. INTRODUCTION

Molecular graphs can distinguish between structural isomers, compounds which have the same molecular formula but non-isomorphic graphs- such as isopentane and neopentane. On the other hand, the molecular graph normally does not contain any information about the three-dimensional arrangement of the bonds, and therefore cannot distinguish between conformational isomers (such as cis and trans 2-butene) or stereoisomers (such as D- and L-glyceraldehyde).

In some important cases (topological index calculation etc.) the following classical definition is sufficient: molecular graph is connected undirected graph one-to-one corresponded to structural formula of chemical compound so that vertices of the graph

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correspond to atoms of the molecule and edges of the graph correspond to chemical bonds between these atoms.

In the fields of chemical graph theory, molecular topology, and mathematical chemistry, a topological index also known as a connectivity index is a type of a molecular descriptor that is calculated based on the molecular graph of a chemical compound. Topological indices are numerical parameters of a graph which characterize its topology and are usually graph invariant. Topological indices are used for example in the development of quantitative structure-activity relationships (QSARs) in which the biological activity or other properties of molecules are correlated with their chemical structure. The simplest topological indices do not recognize double bonds and atom types (C, N, O etc.) and ignore hydrogen atoms ("hydrogen suppressed") and defined for connected undirected molecular graphs only. More sophisticated topological indices also take into account the hybridization state of each of the atoms contained in the molecule. Hundreds of indices were introduced. The Hosoya index is the first topological index recognized in chemical graph theory, and it is often referred to as the topological index. Other examples include the Wiener index, Randić's molecular connectivity index, Balaban's J index, and the TAU descriptors [12].

Let G be a molecular graph. Two vertices of G , connected by an edge, are said to be adjacent. The number of vertices of G , adjacent to a given vertex v , is the degree of this vertex, and will be denoted by $d(v)$. Gutman [5] introduced the following general form for topological indices:

$$TI_s = TI_s(G) = \sum_{uv \in E(T)} F(d(u), d(v)),$$

where the summation goes over all pairs of adjacent nodes u, v of molecular graph G , and where $F = F(x, y)$ is an appropriately chosen function. In particular, $F(x, y) = (xy)^{-1/2}$ for Randić index, $F(x, y) = x + y$ for the first Zagreb index, $F(x, y) = xy$ for the second Zagreb index, $F(x, y) = |x - y|$ for the third Zagreb index, $F(x, y) = (xy)^\lambda$ ($\lambda \in \mathbf{R}$) for the second variable Zagreb index, $F(x, y) = ((x+y-2)(xy)^{-1})^{1/2}$ for the ABC index, $F(x, y) = (xy(x+y-2)^{-1})^3$, for the augmented Zagreb index, $F(x, y) = 2\sqrt{xy}(x+y)^{-1}$ for the geometric-arithmetic index, $F(x, y) = 2(x+y)^{-1}$ for the harmonic index and $F(x, y) = (x+y)^{-1/2}$ for the sum-connectivity index.

Todeschini *et al.* [15,16] proposed that multiplicative variants of molecular structure descriptors be considered. Thus we have the following general form for topological indices:

$$TI_p = TI_p(G) = \prod_{uv \in E(T)} F(d(u), d(v)).$$

When this idea is applied to Zagreb indices, one arrives at their multiplicative versions $\Pi_1(G)$ and $\Pi_2(G)$, defined as $\Pi_1(G) = \prod_{v \in V(G)} (d(v))^2$ and $\Pi_2(G) = \prod_{uv \in E(G)} d(u)d(v)$ [3, 4]. Réti and Gutman [14] provided lower and upper bounds for Π_1 and Π_2 of a connected graph in terms of the number of vertices, number of edges, and the ordinary, additive Zagreb indices M_1 and M_2 . Let T_n be the set of trees with n vertices. Gutman [6] determined the elements of T_n , extremal w.r.t. Π_1 and Π_2 . Iranmanesh *et al.* [7] computed these indices for link and splice of graphs. In continuation, with use these graphs, they computed the first and the second multiplicative Zagreb indices for a class of dendrimers. Liu and Zhang [13] introduced several sharp upper bounds for Π_1 -index in terms of graph parameters including the order, size, radius, Wiener index and eccentric distance sum, and upper bounds for Π_2 -index in terms of graph parameters including the order, size, the first Zagreb index, the first Zagreb coindex and degree distance. Xu and Hua [18] obtained a unified approach to characterize extremal (maximal and minimal) trees, unicyclic graphs and bicyclic graphs with respect to multiplicative Zagreb indices, respectively. Recently, Wang and Wei studied these indices in k -trees [17].

Another multiplicative version of the first Zagreb index is defined as $\Pi_3(G) = \prod_{uv \in E(G)} (d(u) + d(v))$ and is named as the multiplicative sum Zagreb index. Eliasi *et al.* [2] proved that among all connected graphs with a given number of vertices, the path has minimal Π_3 . They also determined the trees with the second-minimal Π_3 . Kazemi [11] studied Π_1, Π_2 and Π_3 in random molecular graphs with tree structure. He gave the lower and upper bounds related to the moments of these indices.

We introduce the modified multiplicative sum Zagreb index, defined as

$$\Pi_4(G) = \prod_{uv \in E(G)} (d(u) + d(v))^{d(u)d(v)},$$

and study it in random molecular graphs with tree structure. An illustrative example is provided in Figure 1.

2. EVOLUTION PROCESS

The structures of many molecules such as dendrimers and acyclic molecules are tree like. We present the following evolution process for random trees of order n , which turns out to be appropriate when studying the multiplicative Zagreb indices of molecular graphs with tree structure [10].

Every order- n tree can be obtained uniquely by attaching n th node to one of the $n-1$ nodes in a tree of order $n-1$. It is of particular interest in applications to assume the random tree model and to speak about a random tree with n nodes, which means that all

trees of order n are considered to appear equally likely. Equivalently one may describe random trees via the following tree evolution process, which generates random trees of arbitrary order n . At step 1 the process starts with a node. At step i the i th node is attached to any previous node v of the already grown tree T of order $i-1$ with probability $p_i(v) = 1/(i-1)$. For applicability of our own results and specially connection with the chemical relevance, see [9].

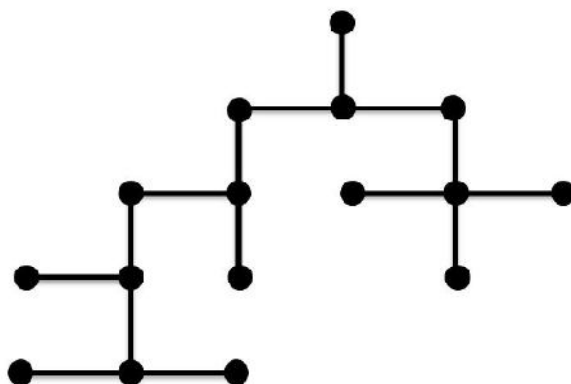


Figure 1. A molecular graph with $\Pi_1 = 6718464$, $\Pi_2 = 8707129344$, $\Pi_3 = 14400000000$ and $\Pi_4 = 4 \times 10^{51}$.

Let $d(v,n)$ denote the degree of node v in our structure of order n . It is obvious that $1 \leq d(v,n) \leq n-1$. We define \mathbf{B}_n to be the sigma-field generated by the first n stages of the random molecular graphs with tree structure. Let \mathbf{T}_n be the set of trees with order n . Then by definition of the multiplicative Zagreb indices for $k \geq 1$ and $i = 1, 2, 3$ [11],

$$\frac{\Pi_i(\mathbf{T}_n)^k}{\Pi_i(\mathbf{T}_{n-1})^k} = f_{\Pi_i}(d(U, n-1))^k, \quad (1)$$

where U is independent of \mathbf{B}_{n-1} . Let $\{y_1, \dots, y_k\}$ be the neighborhood of the vertex U . Also

$$f_{\Pi_i}(d(U, n-1)) = \begin{cases} \left(\frac{d(U, n-1)+1}{d(U, n-1)} \right)^2, & \text{for } i = 1 \\ \left(\frac{d(U, n-1)+1}{d(U, n-1)} \right)^{d(U, n-1)} \times (d(U, n-1)+1), & \text{for } i = 2 \\ \prod_{k=1}^{d(U, n-1)} \frac{d(U, n-1) + d(y_k, n-1) + 1}{d(U, n-1) + d(y_k, n-1)}, & \text{for } i = 3. \end{cases}$$

It is obvious that

$$a_{\Pi_i} := \min f_{\Pi_i}(d(U, n-1))^k = \begin{cases} \left(\frac{n-2}{n-3}\right)^{2k}, & \text{for } i=1 \\ 4^k, & \text{for } i=2 \\ \left(3\frac{n-1}{n-2}\right)^k, & \text{for } i=3 \end{cases}$$

and

$$d_{\Pi_i} := \max f_{\Pi_i}(d(U, n-1))^k = \begin{cases} 4^k, & \text{for } i=1 \\ \left(\frac{n-2}{n-3}\right)^{k(n-3)} (n-2)^k, & \text{for } i=2 \\ \left(\frac{n-1}{n-2}\right)^{k(n-3)} (n-1)^k, & \text{for } i=3. \end{cases}$$

Theorem 1 [11] Let $\mathbf{E}(\Pi_i(T_n)^k)$ ($k \geq 1, i=1,2,3$) be the k th moment of $\Pi_i(T_n)$ of a molecular graph T_n with tree structure of order n . Then for $n \geq 5$,

$$(n-2)^{2k} \leq \mathbf{E}(\Pi_1(T_n)^k) \leq 4^{k(n-2)} \quad (a.e.),$$

$$4^{k(n-2)} \leq \mathbf{E}(\Pi_2(T_n)^k) \leq (n-2)^{(n-2)k}, \quad (a.e.),$$

$$\left(\frac{2}{9}3^n(n-1)\right)^k \leq \mathbf{E}(\Pi_3(T_n)^k) \leq 2^k(n-1)^{k(n-2)}, \quad (a.e.).$$

3. MAIN RESULTS

3.1 RATIO OF THE MULTIPLICATIVE ZAGREB INDICES

In this section, we obtain lower and upper bounds for the moments of the ratio of the multiplicative Zagreb indices (Π_1, Π_2 and Π_3).

Theorem 2 Suppose

$$\Pi_{i,j,k}(T_n) = \mathbf{E}\left(\frac{\Pi_i(T_n)}{\Pi_j(T_n)}\right)^k, \quad i \neq j, \quad i, j = 1, 2, 3.$$

Then

$$\Pi_{1,2,k}(T_n) \geq \left(\frac{n-2}{(n-3)^2}\right)^{k(n-2)}, \quad \Pi_{1,3,k}(T_n) \geq \frac{1}{2^k} \left(\frac{n-2}{(n-3)(n-1)^{\frac{1}{2}}}\right)^{2k(n-2)},$$

$$\begin{aligned} \Pi_{2,1,k}(T_n) \geq 1, \Pi_{2,3,k}(T_n) &\geq \frac{1}{2^k} \left(\frac{4}{n-1} \right)^{k(n-2)}, \\ \Pi_{3,1,k}(T_n) \geq 2^k \left(\frac{3n-1}{4n-2} \right)^{k(n-2)}, \Pi_{3,2,k}(T_n) &\geq 2^k \left(\frac{3(n-1)}{(n-2)^2} \right)^{k(n-2)}. \end{aligned}$$

Proof. It is obvious that for $i = 1, 2, 3$, $\Pi_i(T_n)^k > \Pi_i(T_{n-1})^k$. Then

$$\begin{aligned} \Pi_{i,j,k}(T_n) &= \mathbf{E} \left(\mathbf{E} \left(\frac{\Pi_i(T_n)^k}{\Pi_j(T_n)^k} \mid \mathbf{B}_{n-1} \right) \right) \\ &> \mathbf{E} \left(\mathbf{E} \left(\frac{\Pi_i(T_{n-1})^k}{\Pi_j(T_n)^k} \mid \mathbf{B}_{n-1} \right) \right) \\ &= \mathbf{E} \left(\Pi_i(T_{n-1})^k \mathbf{E} \left(\frac{1}{\Pi_j(T_n)^k} \mid \mathbf{B}_{n-1} \right) \right) \\ &\geq \mathbf{E} \left(a_{\Pi_i} \Pi_i(T_{n-2})^k \mathbf{E} \left(\frac{1}{\Pi_j(T_n)^k} \mid \mathbf{B}_{n-1} \right) \right) \\ &\geq \dots \geq \mathbf{E} \left(a_{\Pi_i}^{n-2} \Pi_i(T_2)^k \mathbf{E} \left(\frac{1}{\Pi_j(T_n)^k} \mid \mathbf{B}_{n-1} \right) \right) \\ &= a_{\Pi_i}^{n-2} b_{\Pi_i}^k \mathbf{E} \left(\mathbf{E} \left(\frac{1}{\Pi_j(T_n)^k} \mid \mathbf{B}_{n-1} \right) \right), \quad b_{\Pi_i} = \Pi_i(T_2) \\ &= a_{\Pi_i}^{n-2} b_{\Pi_i}^k \mathbf{E} \left(\frac{1}{\Pi_j(T_n)^k} \right), \end{aligned}$$

where $b_{\Pi_1} = b_{\Pi_2} = 1$, $b_{\Pi_3} = 2$. By Jensen's inequality [1],

$$\Pi_{i,j,k}(T_n) \geq a_{\Pi_i}^{n-2} b_{\Pi_i}^k \frac{1}{\mathbf{E}(\Pi_j(T_n)^k)},$$

and proof is completed by Theorem 1.

Corollary 1 Suppose $m \neq n (m, n \in \mathbf{N})$ and

$$\Pi_{i,j,k}(T_m, T_n) = \mathbf{E} \left(\frac{\Pi_i(T_n)}{\Pi_j(T_m)} \right)^k, \quad i, j = 1, 2, 3.$$

Then

$$\Pi_{1,1,k}(T_m, T_n) \geq \left(\frac{n-2}{n-3} \right)^{2k(n-2)} 4^{-k(m-2)}, \Pi_{2,2,k}(T_m, T_n) \geq \frac{4^{k(n-2)}}{(m-2)^{k(m-2)}},$$

$$\begin{aligned} \Pi_{3,3,k}(T_m, T_n) &\geq \left(\frac{3(n-1)}{n-2}\right)^{k(n-2)} (m-1)^{-k(m-2)}, \\ \Pi_{1,2,k}(T_m, T_n) &\geq \left(\frac{n-2}{n-3}\right)^{2k(n-2)} (m-2)^{-k(m-2)}, \\ \Pi_{1,3,k}(T_m, T_n) &\geq \frac{1}{2^k} \left(\frac{n-2}{n-3}\right)^{2k(n-2)} (m-1)^{-k(m-2)}, \\ \Pi_{2,1,k}(T_m, T_n) &\geq 4^{n-m}, \quad \Pi_{2,3,k}(T_m, T_n) \geq \frac{4^{k(n-2)}}{2^k (m-1)^{k(m-2)}}, \\ \Pi_{3,1,k}(T_m, T_n) &\geq 2^k \left(3 \frac{n-1}{n-2}\right)^{k(n-2)} 4^{-k(m-2)}, \\ \Pi_{3,2,k}(T_m, T_n) &\geq 2^k \left(\frac{3(n-1)}{(n-2)^2}\right)^{k(n-2)} (m-2)^{-k(m-2)}. \end{aligned}$$

With this approach, we can obtain the sharp lower bounds for different values of k .

Theorem 3 Suppose

$$\Pi_{i,j,k}(T_n) = \mathbf{E} \left(\frac{\Pi_i(T_n)}{\Pi_j(T_n)} \right)^k, \quad i \neq j, \quad i, j = 1, 2, 3.$$

Then

$$\begin{aligned} \Pi_{1,2,k}(T_n) &\leq 4^{k(n-2)}, \quad \Pi_{1,3,k}(T_n) \leq \left(\frac{1}{2}\right)^k 4^{k(n-2)}, \\ \Pi_{2,1,k}(T_n) &\leq \left(\frac{n-2}{n-3}\right)^{k(n-3)(n-2)} (n-2)^{k(n-2)}, \\ \Pi_{2,3,k}(T_n) &\leq \left(\frac{1}{2}\right)^k \left(\frac{n-2}{n-3}\right)^{k(n-3)(n-2)} (n-2)^{k(n-2)}, \\ \Pi_{3,1,k}(T_n) &\leq 2^k \left(\frac{n-1}{n-2}\right)^{k(n-3)(n-2)} (n-1)^{k(n-2)}, \\ \Pi_{3,2,k}(T_n) &\leq 2^k \left(\frac{n-1}{n-2}\right)^{k(n-3)(n-2)} (n-1)^{k(n-2)}. \end{aligned}$$

Proof. We have [11]:

$$\mathbf{E}(\Pi_1(T_n)^k | \mathbf{B}_{n-1}) \leq d_{\Pi_1} \Pi_1(T_{n-1})^k, \quad (a.e.),$$

$$\mathbf{E}(\Pi_2(T_n)^k | \mathbf{B}_{n-1}) \leq d_{\Pi_2} \Pi_2(T_{n-1})^k, \quad (a.e.),$$

$$\mathbf{E}(\Pi_3(T_n)^k | \mathbf{B}_{n-1}) \leq d_{\Pi_3} \Pi_3(T_{n-1})^k, \quad (a.e.). \quad (2)$$

Thus

$$\begin{aligned}
 \Pi_{i,j,k}(T_n) &= \mathbf{E} \left(\mathbf{E} \left(\frac{\Pi_i(T_n)^k}{\Pi_j(T_n)^k} \mid \mathbf{B}_{n-1} \right) \right) \\
 &\leq \mathbf{E} \left(\mathbf{E} \left(\frac{\Pi_i(T_n)^k}{\Pi_j(T_{n-1})^k} \mid \mathbf{B}_{n-1} \right) \right) \\
 &= \mathbf{E} \left(\frac{1}{\Pi_j(T_{n-1})^k} \mathbf{E}(\Pi_i(T_n)^k \mid \mathbf{B}_{n-1}) \right) \\
 &\leq d_{\Pi_i} \mathbf{E} \left(\frac{\Pi_i(T_{n-1})^k}{\Pi_j(T_{n-1})^k} \right) \\
 &\leq d_{\Pi_i} \mathbf{E} \left(\frac{\Pi_i(T_{n-1})^k}{\Pi_j(T_{n-2})^k} \right) \\
 &= d_{\Pi_i} \mathbf{E} \left(\mathbf{E} \left(\frac{\Pi_i(T_{n-1})^k}{\Pi_j(T_{n-2})^k} \mid \mathbf{B}_{n-2} \right) \right) \\
 &= d_{\Pi_i} \mathbf{E} \left(\frac{1}{\Pi_j(T_{n-2})^k} \mathbf{E}(\Pi_i(T_{n-1})^k \mid \mathbf{B}_{n-2}) \right) \\
 &\leq d_{\Pi_i}^2 \mathbf{E} \left(\frac{\Pi_i(T_{n-2})^k}{\Pi_j(T_{n-2})^k} \right) \\
 &\leq \dots \leq d_{\Pi_i}^{n-2} \mathbf{E} \left(\frac{\Pi_i(T_2)^k}{\Pi_j(T_2)^k} \right) \\
 &= d_{\Pi_i}^{n-2} \Pi_{i,j,k}(T_2),
 \end{aligned}$$

where

$$\Pi_{1,3,k}(T_2) = \Pi_{2,3,k}(T_2) = (1/2)^k,$$

$$\Pi_{3,1,k}(T_2) = \Pi_{3,2,k}(T_2) = 2^k,$$

$$\Pi_{2,1,k}(T_2) = \Pi_{1,2,k}(T_2) = 1.$$

Now, the proof is completed by inequalities (2).

We can introduce the upper bounds similar to Corollary 1.

Corollary 2 *Let $i, j, k, l = 1, 2, 3$, $n, p \geq 5$ and*

$$\Pi_{i,j,k,l}(T_n, T_p) = \mathbf{E} \left(\frac{\Pi_i(T_n) \Pi_k(T_p)}{\Pi_j(T_n) \Pi_l(T_p)} \right).$$

Let $r, s \in [1, \infty]$ with $1/r + 1/s = 1$. By Holder's inequality,

$$\Pi_{i,j,k,l}(T_n, T_p) \leq \Pi_{i,j,r}(T_n)^{\frac{1}{r}} \Pi_{k,l,s}(T_p)^{\frac{1}{s}}.$$

For example,

$$\Pi_{1,2,3,2}(T_5, T_6) \leq \Pi_{1,2,r}(T_5)^{\frac{1}{r}} \Pi_{3,2,s}(T_6)^{\frac{1}{s}} \leq \frac{5^{16}}{4^9}.$$

3.2 MODIFIED MULTIPLICATIVE SUM ZAGREB INDEX

For a path P_n ,

$$\Pi_4(P_n) = 256(n-3) + 18, \quad n \geq 3$$

and for a star S_n ,

$$\Pi_4(S_n) = n^{n-1}(n-1), \quad n \geq 2$$

Lemma 1 Let

$$f(x, y_1, \dots, y_x) = (x+2)^{x+1} \prod_{i=1}^x \frac{(x+y_i+1)^{(x+1)y_i}}{(x+y_i)^{xy_i}}, \quad x, y_i = 1, 2, 3, \dots, n-3.$$

Then

$$f(1, 1, \dots, 1) \leq f(x, y_1, \dots, y_x) \leq f(n-3, n-3, \dots, n-3).$$

Proof. It is enough to note that the function $f(x, y_1, \dots, y_x)$ is increasing in each y_i and x . Let vertex U is uniformly distributed on the vertex set $\{v_1, v_2, \dots, v_{n-1}\}$. Then by definition of the modified multiplicative sum Zagreb index,

$$\begin{aligned} \Pi_4(T_n) &= \Pi_4(T_{n-1})(d(U, n-1) + 2)^{d(U, n-1)+1} \\ &\quad \times \prod_{i=1}^{d(U, n-1)} \frac{(d(U, n-1) + d(y_i, n-1) + 1)^{(d(U, n-1)+1)d(y_i, n-1)}}{(d(U, n-1) + d(y_i, n-1))^{d(U, n-1)d(y_i, n-1)}}, \quad (3) \end{aligned}$$

where U is independent of \mathbf{B}_{n-1} and node y_i is the neighborhood of the vertex U .

Theorem 4 Let $\mathbf{E}(\Pi_4(T_n)^k)$ ($k \geq 1$) be the k th moment of $\Pi_4(T_n)$ of a molecular graph T_n with tree structure of order n . Then for $\mathbf{T}_n \setminus \{P_n, S_n\}$,

$$2^k \left(\frac{81}{2}\right)^{k(n-2)} \leq \mathbf{E}(\Pi_4(T_n)^k) \leq 81^k \prod_{j=3}^{n-1} j^{k(j-1)} \left(\frac{(2j-3)^{j-1}}{(2j-4)^{j-2}}\right)^{k(j-2)^2}, \quad (a.e.). \quad (4)$$

Proof. It is obvious that $\Pi_4(T_{n-1})$ is \mathbf{B}_{n-1} -measurable and the n th vertex is attached to any previous vertex v of the already grown structure T_{n-1} with probability $1/(n-1)$ [8,10]. From Lemma 1 and Equation (3),

$$\mathbf{E}(\Pi_4(T_n)^k | \mathbf{B}_{n-1}) = \mathbf{E}(\Pi_4(T_n)^k | d(v_j, n-1), j = 1, \dots, n-1)$$

$$\begin{aligned} &\geq \frac{\Pi_4(T_{n-1})^k}{n-1} \sum_{j=1}^{n-1} \prod_{i=1}^{d(v_j, n-1)} (d(v_j, n-1) + 2)^{k(d(v_j, n-1)+1)} \frac{(d(v_j, n-1) + 2)^{k(d(v_j, n-1)+1)}}{(d(v_j, n-1) + 1)^{kd(v_j, n-1)}} \\ &\geq \Pi_4(T_{n-1})^k \left(\frac{81}{2}\right)^k, \quad (a.e.) \\ &\geq \dots \geq 2^k \left(\frac{81}{2}\right)^{k(n-2)}, \end{aligned}$$

since $\Pi_4(T_2) = 2$. We can obtain the upper bound from Lemma 1 and $\Pi_4(T_3) = 81$.

Theorem 5 Assume $\Pi_{4,i,k} = \left(\frac{\Pi_4(T_{i+1})}{\Pi_4(T_{i-1})}\right)^k$, for $i \geq 5$ and $k \geq 1$. Then almost everywhere,

$$\left(\frac{81}{2}\right)^{2k} \leq \mathbf{E}(\Pi_{4,i,k}) \leq (i-1)^{k(i-2)} \left(\frac{(2i-5)^{i-2}}{(2i-6)^{i-3}}\right)^{k(i-3)^2} (j-1)^{k(j-2)} \left(\frac{(2j-5)^{j-2}}{(2j-6)^{j-3}}\right)^{k(j-3)^2}.$$

Proof. Suppose $Y_{4,i,k} = \left(\frac{\Pi_4(T_i)}{\Pi_4(T_{i-1})}\right)^k$ for $i \geq 5$. Then $\mathbf{E}(\Pi_{4,i,k}) = \mathbf{E}(Y_{4,i,k} Y_{4,i+1,k})$. Now, from Theorem 4 and the law of the iterated expectation,

$$\begin{aligned} \mathbf{E}(\Pi_{4,i,k}) &= \mathbf{E}(\mathbf{E}(Y_{4,i,k} Y_{4,i+1,k} | \mathbf{B}_i)) \\ &= \mathbf{E}(Y_{4,i,k} \mathbf{E}(Y_{4,i+1,k} | \mathbf{B}_i)), \quad (a.e.) \\ &\geq \left(\frac{81}{2}\right)^k \mathbf{E}(Y_{4,i,k}) \\ &= \left(\frac{81}{2}\right)^k \mathbf{E}(\mathbf{E}(Y_{4,i,k} | \mathbf{B}_{i-1})) \\ &\geq \left(\frac{81}{2}\right)^{2k}. \end{aligned}$$

With this approach, we can obtain the upper bound.

Corollary 3 We have

$$\Pi_{1,4,k}(T_n) \geq \frac{\left(\frac{n-2}{n-3}\right)^{2k(n-2)}}{81^k \prod_{j=3}^{n-1} j^{k(j-1)} \left(\frac{(2j-3)^{j-1}}{(2j-4)^{j-2}}\right)^{k(j-2)^2}},$$

$$\begin{aligned} \Pi_{2,4,k}(T_n) &\geq \frac{4^{k(n-2)}}{81^k \prod_{j=3}^{n-1} j^{k(j-1)} \left(\frac{(2j-3)^{j-1}}{(2j-4)^{j-2}} \right)^{k(j-2)^2}}, \\ \Pi_{3,4,k}(T_n) &\geq \frac{2^k \left(\frac{3(n-1)}{n-2} \right)^{k(n-2)}}{81^k \prod_{j=3}^{n-1} j^{k(j-1)} \left(\frac{(2j-3)^{j-1}}{(2j-4)^{j-2}} \right)^{k(j-2)^2}}, \\ \Pi_{4,1,k}(T_n) &\geq \frac{2^k \left(\frac{81}{2} \right)^{k(n-2)}}{4^{k(n-2)}}, \quad \Pi_{4,2,k}(T_n) \geq \frac{2^k \left(\frac{81}{2} \right)^{k(n-2)}}{(n-2)^{k(n-2)}}, \\ \Pi_{4,3,k}(T_n) &\geq \frac{\left(\frac{81}{2} \right)^{k(n-2)}}{(n-1)^{k(n-2)}}, \quad \Pi_{1,4,k}(T_n) \leq \frac{4^{k(n-2)}}{2^k}, \\ \Pi_{2,4,k}(T_n) &\leq \frac{1}{2^k} \left(\frac{n-2}{n-3} \right)^{k(n-2)(n-3)} (n-2)^{k(n-2)}, \\ \Pi_{3,4,k}(T_n) &\leq \left(\frac{n-1}{n-2} \right)^{k(n-3)(n-2)} (n-1)^{k(n-2)}, \\ \Pi_{4,1,k}(T_n) &\leq 2^k (n-1)^{k(n-2)^2} \left(\frac{(2n-5)^{n-2}}{(2n-6)^{n-3}} \right)^{k(n-3)^2(n-2)}, \\ \Pi_{4,2,k}(T_n) &\leq 2^k (n-1)^{k(n-2)^2} \left(\frac{(2n-5)^{n-2}}{(2n-6)^{n-3}} \right)^{k(n-3)^2(n-2)}, \\ \Pi_{4,3,k}(T_n) &\leq (n-1)^{k(n-2)^2} \left(\frac{(2n-5)^{n-2}}{(2n-6)^{n-3}} \right)^{k(n-3)^2(n-2)}. \end{aligned}$$

since

$$a_{\Pi_4} = \left(\frac{81}{2} \right)^k, \quad b_{\Pi_4} = 2, \quad d_{\Pi_4} = (n-1)^{k(n-2)} \left(\frac{(2n-5)^{n-2}}{(2n-6)^{n-3}} \right)^{k(n-3)^2}.$$

Also, $\Pi_{1,4,k}(T_2) = \Pi_{2,4,k}(T_2) = (1/2)^k$, $\Pi_{4,1,k}(T_2) = \Pi_{4,2,k}(T_2) = 2^k$, $\Pi_{3,4,k}(T_2) = \Pi_{4,3,k}(T_2) = 1$.

Theorem 6 Let τ be a finite stopping time for $\left\{ \frac{\Pi_1(T_n)^k}{\mathbf{E}(\Pi_4(T_n)^k)}, \mathbf{B}_n \right\}_{n \geq 5}$. Then

$$\mathbf{E} \left(\frac{\Pi_1(T_\tau)^k}{\mathbf{E}(\Pi_4(T_\tau)^k)} \right) \leq 1.$$

Also, for $\lambda \geq 0$,

$$P\left(\sup_{n \geq 5} \frac{\Pi_1(T_n)^k}{\mathbf{E}(\Pi_4(T_n)^k)} \geq \lambda\right) \leq \frac{1}{\lambda}.$$

Proof. We have

$$\begin{aligned} \mathbf{E}\left(\frac{\Pi_1(T_n)^k}{\mathbf{E}(\Pi_4(T_n)^k)} \mid \mathbf{B}_{n-1}\right) &= \frac{\mathbf{E}(\Pi_1(T_n)^k \mid \mathbf{B}_{n-1})}{\mathbf{E}(\Pi_4(T_n)^k)} \\ &\leq \frac{4^k \Pi_1(T_{n-1})^k}{\left(\frac{81}{2}\right)^k \mathbf{E}(\Pi_4(T_{n-1})^k)}, \quad (a.e.) \\ &\leq \frac{\Pi_1(T_{n-1})^k}{\mathbf{E}(\Pi_4(T_{n-1})^k)}, \quad (a.e.). \end{aligned}$$

Then $\left\{\frac{\Pi_1(T_n)^k}{\mathbf{E}(\Pi_4(T_n)^k)}, \mathbf{B}_n\right\}_{n \geq 5}$ is a supermartingale. Also, $\frac{\Pi_1(T_n)^k}{\mathbf{E}(\Pi_4(T_n)^k)} > 0$. Proof is completed by Doob's supermartingale inequality [1].

Theorem 7 Suppose $5 \leq m < n$. For $i = 1, 2, 3, 4$ and $k_1, k_2 \geq 1$,

$$\frac{\mathbf{E}(\Pi_i(T_n)^{k_1} \Pi_j(T_m)^{k_2})}{\mathbf{E}(\Pi_i(T_m)^{k_1} \Pi_j(T_m)^{k_2})} \geq a_{\Pi_i},$$

where $a_{\Pi_i} = \min f_{\Pi_i}(d(U, n-1))^{k_1}$.

Proof. If $m < n$, then $\Pi_i(T_m) \leq \Pi_i(T_{n-1})$ and $\mathbf{B}_m \subseteq \mathbf{B}_{n-1}$. Then

$$\begin{aligned} \mathbf{E}(\Pi_i(T_n)^{k_1} \Pi_j(T_m)^{k_2}) &= \mathbf{E}(\mathbf{E}(\Pi_i(T_n)^{k_1} \Pi_j(T_m)^{k_2} \mid \mathbf{B}_m)) \\ &= \mathbf{E}(\Pi_j(T_m)^{k_2} \mathbf{E}(\Pi_i(T_n)^{k_1} \mid \mathbf{B}_m)) \\ &= \mathbf{E}(\Pi_j(T_m)^{k_2} \mathbf{E}(\mathbf{E}(\Pi_i(T_n)^{k_1} \mid \mathbf{B}_{n-1}) \mid \mathbf{B}_m)) \\ &\geq \mathbf{E}(\Pi_j(T_m)^{k_2} \mathbf{E}(a_{\Pi_i} \Pi_i(T_{n-1})^{k_1} \mid \mathbf{B}_m)) \\ &\geq a_{\Pi_i} \mathbf{E}(\Pi_i(T_m)^{k_1} \Pi_j(T_m)^{k_2}), \end{aligned}$$

since by [1, Theorem 5.5.10],

$$\mathbf{E}(\mathbf{E}(\Pi_i(T_n) \mid \mathbf{B}_m) \mid \mathbf{B}_{n-1}) = \mathbf{E}(\Pi_i(T_n) \mid \mathbf{B}_m) = \mathbf{E}(\mathbf{E}(\Pi_i(T_n) \mid \mathbf{B}_{n-1}) \mid \mathbf{B}_m) \quad (a.e.).$$

For example,

$$\mathbf{E}(\Pi_4(T_n) \Pi_4(T_m)) \geq 2 \left(\frac{81}{2}\right)^{m-1}.$$

Suppose $5 \leq m < n$ and $r, s \in [1, \infty]$ with $1/r + 1/s = 1$. Then for $i = 1, 2, 3, 4$ and $k_1, k_2 \geq 1$,

$$\mathbf{E}(\Pi_i(T_n)^{k_1} \Pi_j(T_m)^{k_2}) \leq (\mathbf{E}(\Pi_i(T_n)^{k_1 r}))^{\frac{1}{r}} (\mathbf{E}(\Pi_j(T_m)^{k_2 s}))^{\frac{1}{s}}, \quad (a.e.)$$

This bound is an immediate consequence of Holder's inequality. Let

$\Pi_m(T_n) = \sum_{i=1}^m \Pi_i(T_n), 1 \leq m \leq 4$. Then for $r > 1$,

$$\mathbf{E}(\Pi_m(T_n))^r \leq m^{r-1} \sum_{i=1}^m \mathbf{E}(\Pi_i(T_n))^r.$$

For example, $\mathbf{E}((\Pi_1(T_n) + \Pi_3(T_m))^2) \leq 2(4^{2(n-2)} + (m-2)^{2(m-2)})$.

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The Ratio and Product of the Multiplicative Zagreb Indices

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نسبت و ضرب شاخص‌های زاگرب ضربی

ادیتور رابط : سندی کلاوزر

چکیده

شاخص زاگرب ضربی اول $\Pi_1(G)$ برابر حاصل ضرب توان دوم درجه‌ها و شاخص زاگرب ضربی دوم $\Pi_2(G)$ برابر حاصل ضرب درجه زوج رؤوس مجاور گراف مولکولی G است. همچنین، شاخص زاگرب جمعی-ضربی $\Pi_3(G)$ برابر ضرب مجموع درجه زوج رؤوس مجاور G است. در این مقاله، یک نسخه جدید از شاخص زاگرب جمعی-ضربی معرفی و گشتاورهای نسبت و ضرب همه شاخص‌ها در یک گراف مولکولی به طور تصادفی انتخاب شده با ساختار درختی از مرتبه n مطالعه می‌شود. همچنین، یک زیرمارتینگل بر اساس نابرابری زیرمارتینگلی دوب معرفی می‌شود.

لغات کلیدی: گراف مولکولی با ساختار درختی، شاخص زاگرب ضربی، گشتاور، نابرابری زیرمارتینگلی دوب.