



Contents lists available at ScienceDirect

Discrete Applied Mathematics

journal homepage: www.elsevier.com/locate/dam

Note on the multiplicative Zagreb indices

Ramin Kazemi

Department of Statistics, Imam Khomeini International University, Qazvin, Iran

ARTICLE INFO

Article history:

Received 9 November 2014

Received in revised form 21 June 2015

Accepted 23 June 2015

Available online xxxx

Keywords:

The multiplicative Zagreb indices

Moments

Probability generating function

Doob's supermartingale inequality

ABSTRACT

The first and second multiplicative Zagreb indices of a graph G are

$$\Pi_1(G) = \prod_{v \in V(G)} (d(v))^2$$

and

$$\Pi_2(G) = \prod_{uv \in E(G)} d(u)d(v),$$

respectively. Eliasi et al. (2012) introduced a multiplicative version of the first Zagreb index, defined as

$$\Pi_1^*(G) = \prod_{uv \in E(G)} (d(u) + d(v))$$

and Xu and Hua (2012) named it as the multiplicative sum Zagreb index. In this paper, we study the multiplicative Zagreb indices of molecular graphs with tree structure. More precisely, we obtain the bounds for the moments and the probability generating function of these indices in a randomly chosen molecular graph with tree structure of order n .

© 2015 Elsevier B.V. All rights reserved.

1. Introduction

Let G be a molecular graph. The vertex and edge sets of a graph G are denoted by $V(G)$ and $E(G)$, respectively. 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 $d(v)$. The degree-based graph invariants $M_1(G)$ and $M_2(G)$, called Zagreb indices, were introduced more than thirty years ago by Gutman and Trinajstić [6]. For their main properties, chemical applications, and further references see [7]. For some recent mathematical results of these indices, see [2,4,13]. It is known that

$$M_1(G) = \sum_{v \in V(G)} (d(v))^2$$

and

$$M_2(G) = \sum_{uv \in E(G)} d(u)d(v).$$

E-mail address: r.kazemi@SCI.ikiu.ac.ir.<http://dx.doi.org/10.1016/j.dam.2015.06.028>

0166-218X/© 2015 Elsevier B.V. All rights reserved.

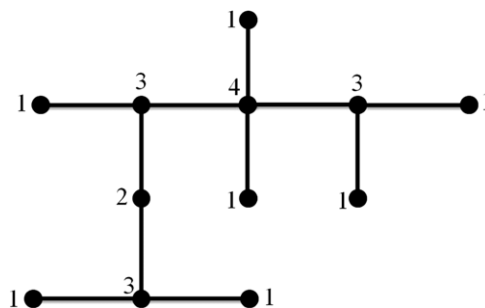


Fig. 1. [12] A molecular graph with its node degrees indicated. In this graph, $\Pi_1 = 46656$, $\Pi_2 = 20155392$ and $\Pi_1^* = 31360000$.

Todeschini et al. [17,18] proposed that multiplicative variants of molecular structure descriptors be considered. 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

$$\Pi_2(G) = \prod_{uv \in E(G)} d(u)d(v).$$

Eliasi et al. [3] considered a multiplicative version of M_1 defined as

$$\Pi_1^*(G) = \prod_{uv \in E(G)} (d(u) + d(v)).$$

They proved that among all connected graphs with a given number of vertices, the path has minimal Π_1^* . They also determined the trees with the second-minimal Π_1^* . Réti and Gutman [16] 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 \mathcal{T}_n be the set of trees with n vertices. Gutman [5] determined the elements of \mathcal{T}_n , extremal w.r.t. Π_1 and Π_2 . Iranmanesh et al. [8] computed these indices for link and splice of graphs. In continuation, with the use of these graphs, they computed the first and the second multiplicative Zagreb indices for a class of dendrimers. Liu and Zhang [14] 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 [20] 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 [19].

This paper attempts to answer the question—What are the expected values of the multiplicative Zagreb indices of a randomly chosen molecular graph with tree structure (of order n)? Since we only know that $\sum_{v \in V(T)} d(v) = 2(n - 1)$, it is impossible to find the exact expected values of these indices. Thus, it is desirable to give the lower and upper bounds for these indices, instead.

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 [12].

Evolution process: 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 $p_i(v) = \frac{1}{i-1}$. For applicability of our own results and specially connection with the chemical relevance, see [10]. An illustrative example is provided in Fig. 1.

For vertices $v, u \in V(G)$, the distance $d(v, u)$ is defined as the length of a shortest path between v and u in G . The eccentric connectivity index of the molecular graph G , $\xi^c(G)$, is defined as $\xi^c(G) = \sum_{v \in V(G)} d(v) \text{ecc}(v)$, where $\text{ecc}(v) = \max\{d(x, v) | x \in V(G)\}$. Let $M_1(T_n)$ and $\xi^c(T_n)$ be the first Zagreb index and the eccentric connectivity index of a random molecular graph T_n with tree structure of order n , respectively. By using the above evolution process, Kazemi [9,10] showed that for $n \geq 2$,

$$\mathbf{E}(M_1(T_n)) = 6n + \mathcal{O}(\log n),$$

$$\mathbf{Var}(M_1(T_n)) = 8n + \mathcal{O}(\log^2 n),$$

$$\mathbf{E}(\xi^c(T_n)) = 3n + \mathcal{O}(\log n),$$

$$\mathbf{Var}(\xi^c(T_n)) = 8n + \mathcal{O}(\log^2 n).$$

Download English Version:

<https://daneshyari.com/en/article/6872032>

Download Persian Version:

<https://daneshyari.com/article/6872032>

[Daneshyari.com](https://daneshyari.com)