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On the First Variable Zagreb Index

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ABSTRACT

The first variable Zagreb index of graph G is defined as $M_1^{\lambda}(G) = \sum_{x\in V(G)} d(v)^{2\lambda}$, where λ is a real number and $d(v)$ is the degree of vertex v. In this paper, some lower and upper bounds for the expected value and distribution function of this index in random increasing trees (recursive trees, plane-oriented recursive trees and binary increasing trees) are given.

1. INTRODUCTION

The concept of the variable molecular descriptors was proposed as an alternative way of characterizing heteroatoms in molecules, but also to assess the structural differences, such as, for example, the relative role of carbon atoms of acyclic and cyclic parts in alkyl cycloalkanes. The idea behind the variable molecular descriptors is that the variables are determined during the regression so that the standard error of estimate for a studied property is as small as possible. Several molecular descriptors, have already been generalized in their variable forms, but here we will only pay attention to first Zagreb index. This index has been used to study molecular complexity, chirality, ZE-isomerism and hetero-systems. Overall, Zagreb indices exhibit a potential applicability for deriving multi-linear regression models [2].

The first variable Zagreb index of graph G is defined by

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$$M_1^{\lambda} = M_1^{\lambda}(G) = \sum_{v \in V(G)} d(v)^{2\lambda}, \tag{1}$$

where λ is a real number and $d(v)$ is the degree of vertex v (for example, see [1] for the case $\lambda \in [0,1/2]$).

There are several tree models, namely so called recursive trees, plane-oriented recursive trees (also known as non-uniform recursive trees or heap ordered trees) and binary increasing trees, which turned out to be appropriate in order to describe the behaviour of a lot of quantities in various applications. All the tree families mentioned above can be considered as so called increasing trees, i.e. labelled trees, where the nodes of a tree of size n are labelled by distinct integers of the set $\{1,2,...,n\}$ in such a way that each sequence of labels along any path starting at the root is increasing. E. g., plane-oriented recursive trees are increasingly labelled ordered trees (= planted plane trees) and binary increasing trees are obtained from (unlabelled) d-ary trees via increasing labellings [2]. We can describe the tree evolution process which generates random trees (of arbitrary size n) of grown trees. This description is a consequence of the considerations made in:
Step 1: The process starts with the root labelled by 1.
Step $i+1$*:* At step $i+1$ the node with label $i+1$ is attached to any previous node v (with out-degree $d^+(v)$) of the already grown tree of size i with probabilities

$$p(v) := \begin{cases} \dfrac{1}{i}, & \textit{for recursive trees} \\ \dfrac{2-d^+(v)}{i+1}, & \textit{for binary increasing trees} \\ \dfrac{d^+(v)+1}{2i-1}, & \textit{for plane-oriented recursive trees.} \end{cases} \tag{2}$$

Since the structures of many molecules are tree like, our interest here is to study the first variable Zagreb index of increasing trees. Several other topological indices of random trees have been studied by many authors. We refer the reader to Kazemi [3, 4, 5] for the first Zagreb, eccentric connectivity index and second Zagreb indices, Kazemi and Meimondari for degree distance and Gutman index [6] and references therein. Our aim in this paper is to consider the expected value and distribution function of the first variable Zagreb index in random trees. In the following, we use the notation R_n^{α} to denote the first variable Zagreb index of an increasing tree of size n with $a \in R$.

2. CASE $\alpha = 2\lambda \in \mathbb{N} \setminus \{1\}$

Let $\alpha = 2\lambda \in \mathbb{N} \setminus \{1\}$ and R_n^{α} be the first variable Zagreb index of an increasing tree of size n. For $\alpha = 1$ (or $\lambda = 1/2$),

$$R_n^1 = \sum_{v \in V(G)} d(v) = 2(n-1).$$

Let $d_{k,n}$ denote the degree of node labeled k in the random tree of size n. Considering the insertion of label n at the nth stage, we obtain

$$\begin{aligned} R_n^\alpha &= R_{n-1}^\alpha + (d_{U_n,n-1}+1)^\alpha - d_{U_n,n-1}^\alpha + 1 \\ &= R_{n-1}^\alpha + \sum_{j=0}^{\alpha-1} \binom{\alpha}{j} d_{U_n,n-1}^j + 1, \end{aligned} \tag{3}$$

where

$$U_n = \sum_{k=1}^{n-1} k\, \mathrm{I}(node\ k\ is\ the\ parent\ of\ node\ n)$$

is uniformly distributed on the set $\{1,2,...,n-1\}$.

Now, let F_n be the sigma-field generated by the first n stages of the increasing trees. By stochastic growth rule of the random increasing trees and definition of conditional expectation,

$$\begin{aligned} \mathbf{E}(R_n^\alpha \mid \mathrm{F}_{n-1}) &= \mathbf{E}(R_n^\alpha \mid d_{k,n-1}, k=1,...,n-1) \\ &= R_{n-1}^\alpha + p(v) \sum_{k=1}^{n-1} \sum_{j=0}^{\alpha-1} \binom{\alpha}{j} d_{k,n-1}^j + 1. \end{aligned} \tag{4}$$

As our first result, we prove the following theorem.

Theorem 1 *We have*

$$\mathbf{E}(R_n^\alpha) \le \begin{cases} n + \sum_{j=3}^{n} \dfrac{(2j-3)^\alpha}{j-1}, & \textit{for recursive trees} \\ n + 2\sum_{j=2}^{n} \dfrac{(2j-3)^\alpha}{j} - 1, & \textit{for binary increasing trees} \\ n + \sum_{j=2}^{n} (2j-3)^{\alpha-1}(j-1) - 1, & \textit{for plane-oriented recursive trees.} \end{cases}$$

Also

$$\mathbf{E}(R_n^\alpha) \ge \begin{cases} n + 2(2^\alpha - 1)\sum_{j=2}^{n} \dfrac{j-2}{j-1}, & \textit{for recursive trees} \\ n + 4(2^\alpha - 1)\sum_{j=2}^{n} \dfrac{j-2}{j} - 1, & \textit{for binary increasing trees} \\ n + 2(2^\alpha - 1)\sum_{j=2}^{n-1} \dfrac{j-2}{2j-3} - 1, & \textit{for plane-oriented recursive trees.} \end{cases}$$

Proof. We have

$$\begin{aligned}
\mathbf{E}(R_n^{\alpha} \mid \mathsf{F}_{n-1}) &= R_{n-1}^{\alpha} + p(v)\sum_{k=1}^{n-1}\sum_{j=0}^{\alpha-1}\binom{\alpha}{j} d_{k,n-1}^{j} + 1 \\
&= R_{n-1}^{\alpha} + p(v)\sum_{j=0}^{\alpha-1}\binom{\alpha}{j}\Big(\sum_{k=1}^{n-1} d_{k,n-1}^{j}\Big) + 1 \\
&\le R_{n-1}^{\alpha} + p(v)\sum_{j=0}^{\alpha}\binom{\alpha}{j}(R_{n-1}^{1})^{j} + 1 \\
&= R_{n-1}^{\alpha} + p(v)(2n-3)^{\alpha} + 1
\end{aligned}$$

and then

$$\mathbf{E}(R_n^{\alpha}) \le \mathbf{E}(R_{n-1}^{\alpha}) + p(v)(2n-3)^{\alpha} + 1.$$

Also,

$$\begin{aligned}
\mathbf{E}(R_n^{\alpha} \mid \mathsf{F}_{n-1}) &\ge R_{n-1}^{\alpha} + p(v)\sum_{j=0}^{\alpha-1}\binom{\alpha}{j} R_{n-1}^{1} + 1 \\
&= R_{n-1}^{\alpha} + p(v)(2(n-2))(2^{\alpha}-1) + 1.
\end{aligned}$$

Now proof is completed by (2) since $R_1^{\alpha} = 0$ and $R_2^{\alpha} = 2$.

For a path P_n, $P_n^{\alpha} := R_n^{\alpha}(P_n) = 2 + 2^{\alpha}(n-2)$ and for a star S_n,

$$S_n^{\alpha} := R_n^{\alpha}(S_n) = (n-1) + (n-1)^{\alpha}.$$

We use the notation $\xrightarrow{D}$ to denote convergence in distribution. If $d_{U_n,n}$ is the degree of a random node in a randomly chosen tree of size n, $d_{U_n,n} \xrightarrow{D} X$ with [7]

$$P(X = k) = \begin{cases} \dfrac{1}{2^{k}}, & \textit{for recursive trees}: k \ge 1 \\ \dfrac{1}{3}, & \textit{for binary increasing trees}: 1 \le k \le 3 \\ \dfrac{2}{3\binom{k+2}{3}}, & \textit{for plane-oriented recursive trees}: k \ge 1. \end{cases} \qquad (5)$$

Thus

$$M(j) := \mathbf{E}(X^j) = \begin{cases} Li_{-j}(\frac{1}{2}), & \textit{for recursive trees} \\ \frac{1}{3}H(j;3), & \textit{for binary increasing trees} \\ 4F(j), & \textit{for plane-oriented recursive trees} \end{cases}$$

where $Li_s(z)$ is the polylogarithm function, $H(p;n) = \sum_{k=1}^{n} k^p$ is the $(p+1)$-th-degree polynomial of n and

$$F(j) = \sum_{k=1}^{\infty} \frac{k^j}{(k+2)(k+1)k}, \quad j \le \alpha - 1.$$

Theorem 2 *For n large enough,*

$$\mathbf{E}(R_n^\alpha) = n + (n-1)\sum_{j=0}^{\alpha-1}\binom{\alpha}{j}M(j) - 1.$$

Proof. If we denote by $X_1 \overset{D}{=} X_2$ the equality in distribution of random variables X_1 and X_2, then from (3),

$$R_{n-1}^\alpha + \sum_{j=0}^{\alpha-1}\binom{\alpha}{j} d_{U_n,n-1}^j + 1 \overset{D}{=} R_{n-1}^\alpha + \sum_{j=0}^{\alpha-1}\binom{\alpha}{j} X^j + 1.$$

Thus

$$\begin{aligned} \mathbf{E}(R_n^\alpha) &= \mathbf{E}(R_{n-1}^\alpha) + \sum_{j=0}^{\alpha-1}\binom{\alpha}{j}\mathbf{E}(X^j) + 1 \\ &= \cdots = n - 1 + (n-1)\sum_{j=0}^{\alpha-1}\binom{\alpha}{j}M(j), \end{aligned}$$

since $R_1^\alpha = 0$.

Corollary 1 *For $\alpha = 2$ in random recursive trees that reduce to the first Zagreb index, we have*

$$\begin{aligned} \mathbf{E}(R_n^2) &= n + (n-1)\sum_{j=0}^{1}\binom{2}{j}\mathrm{Li}_{-j}(\tfrac{1}{2}) - 1 \\ &= n + (n-1)\left(\mathrm{Li}_0(\tfrac{1}{2}) + 2\mathrm{Li}_{-1}(\tfrac{1}{2})\right) - 1 \\ &= n - 1 + (n-1)(1+4) \\ &= 6n - 6, \end{aligned}$$

since

$$\mathrm{Li}_0(z)=\frac{z}{1-z},\quad \mathrm{Li}_{-1}(z)=\frac{z}{(1-z)^2}.$$

Let Δ_n be the maximum degree of any node in a random recursive tree. Szymański [8] proved that

$$\Delta_n \le \log_2 n,$$

for all but $o((n-1)!)$ recursive trees on n nodes. For a binary increasing trees, $\Delta_n \le 3$.

Theorem 3 *i*) *For all but $o((n-1)!)$ recursive trees on n nodes,*

$$\mathbf{E}(R_n^\alpha)\le n+(2^\alpha-1)(\log_2(n-1)!)^{\alpha-1}-1.$$

ii) For binary increasing trees,

$$\mathbf{E}(R_n^\alpha)\le n+(n-1)4^\alpha-1.$$

Proof. i) We have:

$$\begin{aligned}\mathbf{E}(R_n^\alpha)&=\mathbf{E}(R_{n-1}^\alpha)+\mathbf{E}\left(\sum_{j=0}^{\alpha-1}\binom{\alpha}{j}d_{U_n,n-1}^{j}\right)+1\\&\le \mathbf{E}(R_{n-1}^\alpha)+\sum_{j=0}^{\alpha-1}\binom{\alpha}{j}\mathbf{E}(\Delta_{n-1}^{j})+1\\&\le \mathbf{E}(R_{n-1}^\alpha)+(2^\alpha-1)(\log_2(n-1))^{\alpha-1}+1\\&\le\cdots\le n+(2^\alpha-1)(\log_2(n-1)!)^{\alpha-1}-1.\end{aligned}$$

Similarly, we can prove Part (*ii*).

Theorem 4 *For all increasing trees,*

$$\mathbf{E}(R_n^\alpha)\ge P_{n+1}^\alpha-2.$$

Proof. From (3),

$$\begin{aligned}\mathbf{E}(R_n^\alpha)&=\mathbf{E}(R_{n-1}^\alpha)+\mathbf{E}\left(\sum_{j=0}^{\alpha-1}\binom{\alpha}{j}d_{U_n,n-1}^{j}\right)+1\\&=\mathbf{E}(R_{n-1}^\alpha)+\sum_{j=0}^{\alpha-1}\binom{\alpha}{j}\mathbf{E}(d_{U_n,n-1}^{j})+1\\&\ge \mathbf{E}(R_{n-1}^\alpha)+\sum_{j=0}^{\alpha-1}\binom{\alpha}{j}+1,\quad j\ge 0\\&=\cdots=2^\alpha(n-1).\end{aligned}$$

Theorem 5 *Let $F_n^\alpha(r)=P(R_n^\alpha\le r)$ be the distribution function of R_n^α, $r>2(n-1)$ and n be large enough.*

i) For recursive trees,

$$2\left(1-\frac{1}{2^{\sqrt[\alpha]{\frac{r-n}{n-2}}}}\right) < F_n^{\alpha}(r) < 2\left(1-\frac{1}{2^{\sqrt[\alpha-1]{\frac{r-n}{n-2}}}}\right).$$

ii) For binary increasing trees,

$$\frac{\sqrt[\alpha]{\frac{r-n}{n-2}}-1}{3} < F_n^{\alpha}(r) < \frac{\sqrt[\alpha-1]{\frac{r-n}{n-2}}-1}{3}.$$

iii) For plane-oriented recursive trees,

$$\sum_{k=1}^{\sqrt[\alpha]{\frac{r-n}{n-2}}-1}\frac{4}{k(k+1)(k+2)} < F_n^{\alpha}(r) < \sum_{k=1}^{\sqrt[\alpha-1]{\frac{r-n}{n-2}}-1}\frac{4}{k(k+1)(k+2)}.$$

Proof. Suppose $T_\alpha = \sum_{j=0}^{\alpha-1}\binom{\alpha}{j}X^j$. Thus from (3),

$$\begin{aligned}F_n^{\alpha}(r) &= P(R_n^{\alpha} \le r)\\ &= P(R_{n-1}^{\alpha} + T_\alpha + 1 \le r)\\ &= P(T_\alpha \le r - R_{n-1}^{\alpha} - 1)\\ &= \cdots = P((n-2)T_\alpha \le r-n)\\ &= P(T_\alpha \le \frac{r-n}{n-2}).\end{aligned}$$

Also,

$$Z = (1+X)^{\alpha-1} < T_\alpha < W = (1+X)^{\alpha}$$

and

$$F_W(\frac{r-n}{n-2}) < P(T_\alpha \le \frac{r-n}{n-2}) < F_Z(\frac{r-n}{n-2}),$$

where F_Z and F_W are the distribution functions of Z and W, respectively. Now the proof is completed by (5).

3. General Case $\alpha \in R$

Lemma 1 *Let* $f(x) = (x+1)^{\alpha} - x^{\alpha}$, *where* $x > 1$. *Then* $f(x)$ *is decreasing (respectively increasing) for* $0 < \alpha < 1$ *(respectively for* $\alpha < 0$ *or* $\alpha > 1$*).*

Proof. It is enough to note that $f'(x)$ is negative (respectively positive) for $0 < \alpha < 1$ (respectively for $\alpha < 0$ or $\alpha > 1$).

Theorem 6 *Let* $f(n) = (n+1)^{\alpha} - n^{\alpha}$.

i) For $0 < \alpha < 1$,

$$\mathbf{E}(R_n^{\alpha}) \leq \begin{cases} P_n^{\alpha}, & \textit{for recursive trees} \\ n + 2(2^{\alpha} - 1)\sum_{j=2}^{n} \frac{j-1}{j} - 1, & \textit{for binary increasing trees} \\ n + (2^{\alpha} - 1)\sum_{j=3}^{n} \frac{(j-1)(j-2)}{2j-3} - 1, & \textit{for plane-oriented recursive trees} \end{cases}$$

and

$$\mathbf{E}(R_n^{\alpha}) \geq \begin{cases} S_n^{\alpha} + 1, & \textit{for recursive trees} \\ n + 2\sum_{j=2}^{n} \frac{j-1}{j} f(j-2) - 1, & \textit{for binary increasing trees} \\ n + 2\sum_{j=2}^{n} \frac{j-1}{2j-3} f(j-2) - 1, & \textit{for plane-oriented recursive trees} \end{cases}$$

ii) For $\alpha < 0$ or $\alpha > 1$, the presented bounds in Part (i) should be changed by other.

Proof. We have

$$\mathbf{E}(R_n^{\alpha} \mid \mathsf{F}_{n-1}) = R_{n-1}^{\alpha} + p(v)\sum_{k=1}^{n-1} f(d_{k,n-1}) + 1,$$

where $f(1) = 2^{\alpha} - 1$ and $f(n-2) = (n-1)^{\alpha} - (n-2)^{\alpha}$. For Part (i), $f(n-2) < f(1)$ and for Part (ii), $f(1) < f(n-2)$. Now, proof is completed by Lemma 1.

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