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The Eccentric Connectivity Index of Bucket Recursive Trees

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ABSTRACT. If G is a connected graph with vertex set V, then the eccentric connectivity index of G, $\xi^{C}(G)$, is defined as $\sum_{v\in V(G)} deg(v)ecc(v)$ where $deg(v)$ is the degree of a vertex v and $ecc(v)$ is its eccentricity. In this paper we show some convergence in probability and an asymptotic normality based on this index in two classes of random bucket recursive trees.

Keywords: Bucket recursive trees, eccentric connectivity index, convergence in probability, asymptotic normality.

1. INTRODUCTION

Let G be a connected graph with the vertex set $V(G)$ and edge set $E(G)$, respectively. $|V(G)|$, $|E(G)|$ are the number of vertices and edges, respectively. The degree of a vertex $v \in V(G)$ is the number of vertices joining to v and is denoted by $deg(v)$. 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.

In chemistry, a molecular graph represents the topology of a molecule, by considering how the atoms are connected. This can be modeled by a graph, where the points represent the atoms, and the edges symbolize the covalent bonds. Relevant properties of these graph models are then studied, giving rise to numerical graph invariants. The parameters derived from this graph-theoretic model of a chemical structure are being used not only in QSAR studies pertaining to molecular design and pharmaceutical drug design, but also in the environmental hazard assessment of chemicals. Many such graph invariant topological indices have been studied. The first, and most well-known parameter, the Wiener index, was introduced in the late 1940s in

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an attempt to analyze the chemical properties of paraffins (alkanes) (see [12]). This is a distance-based index, whose mathematical properties and chemical applications have been widely researched. Numerous other indices have been defined, and more recently, indices such as the eccentric distance sum, and the adjacency-cum-distance-based eccentric connectivity index have been considered. These topological models have been shown to give a high degree of predictability of pharmaceutical properties, and may provide leads for the development of safe and potent anti-HIV compounds.

The eccentric connectivity index of the molecular graph G, $\xi^c(G)$, was proposed by Sharma, Goswami and Madan (see [2]). It is defined as

$$\xi^c(G) = \sum_{v \in V(G)} deg(v) ecc(v),$$

where $ecc(v) = \max\{d(x,v) \mid x \in V(G)\}$. The references [3, 11, 14] provide properties of the eccentric connectivity index and compare it to other topological indices. Also, an application of the eccentric connectivity index has also been considered in [13].

Trees are defined as connected graphs without cycles. Recursive trees are rooted labelled trees, where the root is labelled by 1 and the labels of all successors of any node v are larger than the label of v [10]. It is of particular interest in applications to assume the random recursive tree model and to speak about a random recursive tree with n nodes, which means that one of the $(n-1)!$ possible recursive trees with n nodes is chosen with equal probability, i.e., the probability that a particular tree with n nodes is chosen is always $1/(n-1)!$. An interesting and natural generalization of random recursive trees has been introduced in [9], and these are called bucket recursive trees. In this model the nodes of a bucket recursive tree are buckets, which can contain up to a fixed integer amount of $b \geq 1$ labels. In this model, the capacity of buckets is fixed. A probabilistic description of random bucket recursive trees is given by a generalization of the stochastic growth rule for ordinary random recursive trees (which is the special instance $b = 1$). In fact, a tree grows by progressive attraction of increasing integer labels: when inserting label $n+1$ into an existing bucket recursive tree containing n labels (i.e., containing the labels $\{1,2,...,n\}$) all n existing labels in the tree compete to attract the label $n+1$, where all existing labels have equal chance to recruit the new label. If the label winning this competition is contained in a node with less than b labels (an unsaturated bucket or node), label $n+1$ is added to this node, otherwise if the winning label is contained in a node with b labels already (a saturated bucket or node), label $n+1$ is attached to this node as a new bucket containing only the label $n+1$. Starting with a single bucket as the root node containing only the label 1, after $n-1$ insertion steps, where the labels $2,3,...,n$ are successively inserted according to this growth rule, results in a so called random bucket recursive tree with n labels and maximal bucket size b. For an existing bucket recursive tree T with n labels, the probability that a certain node $v \in T$ with capacity $1 \leq c(v) \leq b$ attracts the new label $n+1$ is equal to the number of labels contained in v, i.e., $c(v)/n$ (see [9]). The Figure

1 illustrates a bucket recursive tree of order $n = 11$ with maximal bucket size $b = 2$. Kazemi has studied some topological indices in these models [8].

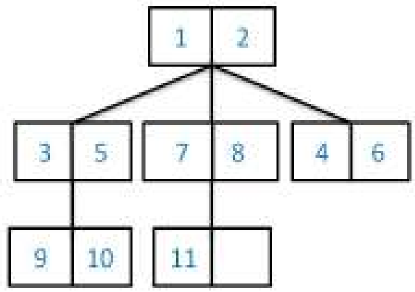

Figure 1: A bucket recursive tree of order 11 with maximal bucket size 2 [8].

It is obvious that the number of nodes (here buckets) in a bucket recursive tree T is less than n for $b > 1$. Thus we can show the order of the tree as a function of n and b. Let $h(b)$ be a real valued function of b, where $h(1) = 0$ and $h(b) \geq 1$ for all $b \geq 2$. Now, we can write the order of the tree as $n - h(b)$, i.e., $|V(T)| = n - h(b)$. We choose the function $h(b)$ in this form for relation between the bucket recursive trees and ordinary recursive trees [9]. Since $\sum_v deg(v) = 2|E(T)|$, thus for our tree of order n,

$$\sum_{v \in V(T)} deg(v) = 2(n - 1 - h(b)). \qquad (1)$$

Another type of bucket recursive tree was recently introduced by Kazemi in 2014 [6]. He has studied branches [7] and the first Zagreb index [5] in these models.

Functional groups are specific groups of atoms or bonds within molecules that are responsible for the characteristic chemical reactions of those molecules. For a connection to chemistry, suppose n atoms in a dendrimer (a repetitively branched molecule) are stochastically labelled with integers 1,2, …, n, then labelled atoms in a functional group can be considered as the labels of a bucket in a bucket recursive tree.

2. Results

Let ξ_n^c be the eccentric connectivity index of a bucket recursive tree T of order n with maximal bucket size b and F_n be the sigma-field generated by the first n stages of these trees. If label n is attached to a leaf with capacity $c(v) < b$, then $\xi_n^c = \xi_{n-1}^c$. But if label n is attached to a saturated bucket (containing the root node), then by the stochastic growth rule of the tree,

$$\begin{aligned}\xi_n^c &= \xi_{n-1}^c - deg(U_{n-1})ecc(U_{n-1})\\ &+ (deg(U_{n-1})+1)ecc(U_{n-1})\\ &+1\cdot(ecc(U_{n-1})+1)\\ &= \xi_{n-1}^c + 2ecc(U_{n-1})+1, \qquad (2)\end{aligned}$$

where $deg(U_{n-1})$ is the degree of the randomly chosen saturated bucket U_{n-1}. From (1), (2) and F_{n-1} −measurability of ξ_{n-1}^c,

$$\begin{aligned}\mathsf{E}(\xi_n^c \mid \mathsf{F}_{n-1}) &= \xi_{n-1}^c + 2b\left(1-\frac{1+h(b)}{n-1}\right)+1\\ &= \xi_{n-1}^c + (2b+1) - 2b\frac{1+h(b)}{n-1}, \qquad (3)\end{aligned}$$

since label n can be attached to buckets with capacity b (a saturated bucket or root node), in a tree of order $n-1$ [1, 9]. Taking the expectation of the relation (3):

$$\mathsf{E}(\xi_n^c) = \mathsf{E}(\xi_{n-1}^c) + (2b+1) - 2b\frac{1+h(b)}{n-1}, \qquad (4)$$

with the initial conditions $\xi_k^c = 0\,(k \le b)$. The recurrence equation (4) leads to

$$\mathsf{E}(\xi_n^c) = n(2b+1) - 2b(1+h(b))(H_{n-1}-H_{b-1}) - b(2b+1), \quad n \ge b, \qquad (5)$$

where $H_n = \sum_{j=1}^n \frac{1}{j}$ is the n th harmonic number [7, 8].

Theorem 1. *For $n \ge b$,*

$$\mathsf{E}(\xi_n^c) = (2b+1)n + \mathsf{O}(\log n),$$
$$\mathsf{V}ar(\xi_n^c) = 8b^2 n + \mathsf{O}(\log^2 n).$$

Proof. The mean is an immediate consequence of (5). Let $Y_k = 0\,(k \le b)$ and for $n \ge b+1$,

$$Y_n = \xi_n^c - \xi_{n-1}^c - (2b+1) + 2b\frac{1+h(b)}{n-1}.$$

Then $\mathsf{E}(Y_n \mid \mathsf{F}_{n-1}) = 0$. From (2),

$$\begin{aligned}\mathsf{E}((\xi_n^c - \xi_{n-1}^c - 1)^2 \mid \mathsf{F}_{n-1}) &= \mathsf{E}(4ecc^2(U_{n-1}))\\ &= 4(\mathsf{V}ar(ecc(U_{n-1})) + \mathsf{E}^2(ecc(U_{n-1})))\\ &= 12b^2\left(1-\frac{1+h(b)}{n-1}\right)^2.\end{aligned}$$

Also,

$$\mathsf{E}((\xi_n^c - \xi_{n-1}^c - 1)^2 \mid \mathsf{F}_{n-1}) = \mathsf{E}\left(\left(Y_n + 2b\left(1 - \frac{1+h(b)}{n-1}\right)\right)^2 \mid \mathsf{F}_{n-1}\right)$$

$$= \mathsf{E}(Y_n^2 \mid \mathsf{F}_{n-1}) + 4b^2\left(1 - \frac{1+h(b)}{n-1}\right)^2.$$

Thus,

$$12b^2\left(1 - \frac{1+h(b)}{n-1}\right)^2 = \mathsf{E}(Y_n^2 \mid \mathsf{F}_{n-1}) + 4b^2\left(1 - \frac{1+h(b)}{n-1}\right)^2. \quad (6)$$

Now, from (6),

$$\mathsf{E}(Y_n^2) = \mathsf{E}(\mathsf{E}(Y_n^2 \mid \mathsf{F}_{n-1}))$$

$$= 8b^2 + \mathsf{O}\left(\frac{\log n}{n}\right), \quad n \ge b+1. \quad (7)$$

Thus

$$\mathsf{V}ar(\xi_n^c) = \sum_{i=b}^{n} \mathsf{E}(Y_i^2) = 8b^2 n + \mathsf{O}(\log^2 n),$$

since for any $b \le i \ne j \le n$, $\mathsf{E}(Y_i Y_j) = 0$ [1].

By Theorem 1 and Chebyshev's inequality, it follows that

$$\frac{\xi_n^c}{\mathsf{E}(\xi_n^c)} \xrightarrow{P} 1$$

and

$$\frac{\xi_n^c}{n} \xrightarrow{P} 2b+1.$$

Also $\sum_{i=b}^{n} i^{-1}(\xi_i^c - \mathsf{E}(\xi_i^c)) = \sum_{i=1}^{n} i^{-1} \sum_{j=b}^{i} Y_j$ and $(H_n - H_{i-1}) \le (H_n - 1)$. Again by Chebyshev's inequality,

$$\sum_{i=b}^{n} (ni)^{-1}(\xi_i^c - \mathsf{E}(\xi_i^c)) \xrightarrow{P} 0.$$

The asymptotic normality is an immediate consequence of the martingale central limit theorem [4], i.e., as $n \to \infty$,

$$\frac{\xi_n^c - (2b+1)n}{\sqrt{8b^2 n}} \xrightarrow{D} N(0,1).$$

With the same approach, we can show that for the bucket recursive trees introduced by Kazemi [6],

$$\mathsf{E}(\xi_n^c) = 3bn + \mathsf{O}(\log n),$$

$$\mathsf{V}ar(\xi_n^c) = (9b^2 - 1)n + \mathsf{O}(\log^2 n),$$

since label n can be attached to buckets with capacities $1, 2, ..., b-1$ or b in a tree of order $n-1$.

Assume $b=1$. Then all results reduce to random recursive trees , i.e.,

$$\mathsf{E}(\xi_n^c) = 3n + \mathsf{O}(\log n),$$

$$\mathsf{V}ar(\xi_n^c) = 8n + \mathsf{O}(\log^2 n),$$

$$n^{-1}\xi_n^c \xrightarrow{P} 3,$$

$$\frac{\xi_n^c - 3n}{\sqrt{8n}} \xrightarrow{D} N(0,1).$$

3. CONCLUSION

The eccentric connectivity index ξ_n^c is a distance-based molecular structure descriptor that was recently used for mathematical modelling of biological activities of diverse nature. In this paper, we showed the first probabilistic analysis of the eccentric connectivity index in two classes of random bucket recursive trees. Through a recurrence equation, the first two moments of ξ_n^c of a random bucket recursive tree of order n, are obtained. The asymptotic normality of the eccentric connectivity index was showed by an application of the martingale central limit theorem. Another topological indices on random trees can be analyzed with this approach.

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