www.combinatorics.ir

Transactions on Combinatorics
ISSN (print): 2251-8657, ISSN (on-line): 2251-8665
Vol. 5 No. 2 (2016), pp. 23-31.

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DEGREE DISTANCE AND GUTMAN INDEX OF INCREASING TREES

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Communicated by Ivan Gutman

Abstract. The Gutman index and degree distance of a connected graph G are defined as

$$\mathrm{Gut}(G)=\sum_{\{u,v\}\subseteq V(G)} d(u)d(v)d_G(u,v),$$

and

$$DD(G)=\sum_{\{u,v\}\subseteq V(G)} (d(u)+d(v))d_G(u,v),$$

respectively, where $d(u)$ is the degree of vertex u and $d_G(u,v)$ is the distance between vertices u and v. In this paper, through a recurrence equation for the Wiener index, we study the first two moments of the Gutman index and degree distance of increasing trees.

1. Introduction

A graph is a collection of points and lines connecting a subset of them. The points and lines of a graph G are also called vertices and edges of the graph and 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 distance between two vertices u and v in a connected graph G is the length of any shortest path between these vertices, and it is denoted by $d_G(u,v)$.

Wiener index, $W(G)$, of a connected graph G is defined as [24]

$$W(G)=\sum_{u,v\in V(G)} d_G(u,v).$$

MSC(2010): Primary: 05C05; Secondary: 60F05.

Keywords: Increasing trees, the Wiener index, the Gutman index, degree distance.

Received: 17 June 2015, Accepted: 21 June 2015.

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In this paper, we are concerned with a variant of the Wiener index called Gutman index [23]. Some authors use alternative name Schultz index of second instead of Gutman index [9]. Throughout this paper, the latter name is used. Another variant of Wiener index is the edge-Wiener index, $W_e(G)$, defined as the sum of the distances between all pairs of edges of a connected graph G:

$$W_e(G) = \sum_{e,f\in E(G)} d_G(e,f),$$

where the distance between two edges is the distance between the corresponding vertices in the line graph of G [6].

Definition 1.1. *The Gutman index of a connected graph G is defined as*

$$\mathrm{Gut}(G) = \sum_{\{u,v\}\subseteq V(G)} d(u)d(v)d_G(u,v).$$

The Gutman index of graphs and its application in chemistry has just recently attracted [2, 20]. Dankelmann et al. [6] presented an asymptotic upper bound for the Gutman index and also established the relation between the edge-Wiener index and Gutman index of graphs. Chen and Liu [3] studied the maximal and minimal Gutman index of unicyclic graphs, and they also determined the minimal Gutman index of bicyclic graphs [4]. Gutman [9] gave the following relation between the Gutman and the Wiener index for a tree T on n vertices,

$$\mathrm{Gut}(T) = 4W(T) - (2n-1)(n-1).$$

For a large number of trees, closed combinatorial expressions for W can be found. The best known of them are

$$W(P_n) = \binom{n+1}{3},\ W(S_n) = (n-1)^2,$$

where P_n is a path (a n-vertex trees with 2 pendent vertices) and S_n is a star (a n-vertex trees with $n-1$ pendent vertices). Thus

$$\mathrm{Gut}(P_n) = \frac{(n-1)(2n^2-4n+3)}{3}$$

and

$$\mathrm{Gut}(S_n) = (2n-3)(n-1).$$

Also, for every tree T_n of order n,

$$\mathrm{Gut}(S_n) \le \mathrm{Gut}(T_n) \le \mathrm{Gut}(P_n). \tag{1.1}$$

There are several tree models, namely so called recursive trees (RT), plane-oriented recursive trees (PORT) and binary increasing trees (BIT), 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 order n are labelled by distinct integers of the set $\{1, 2, \ldots, n\}$ 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 [19]. Figure 1 illustrates a tree of order $n = 7$. One can describe the tree evolution process which generates random trees (of arbitrary order 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 order i with probabilities

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

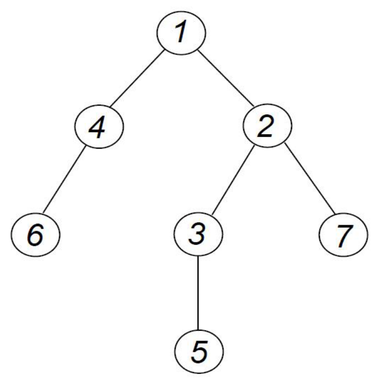

FIGURE 1. A tree of order $n = 7$.

Since the structures of many molecules are tree like, our interest here is to study the Gutman and Schultz indices of random trees. Several other topological indices of random trees have been studied by many authors. We refer the reader to Ali Khan and Neininger [1], Janson [13], Janson and Chassaing [14], and Neininger [21] for the Wiener index, and to Clark and Moon [5], Feng et al. [8], and Hollas [10, 11, 12] for the Randić index and topological indices that depend on the degree of a vertex, Kazemi [15, 16, 17, 18] for the first, second and multiplicative Zagreb indices and eccentric connectivity index, Feng and Hu [7] for the first Zagreb index. In the random tree, $\mathrm{Gut}(T)$ and $W(T)$ become random variables. Thus

$$\mathrm{Gut}(T) \stackrel{D}{=} 4W(T) - (2n-1)(n-1),$$

where $\stackrel{D}{=}$ denotes equality in distribution of the left and right hand side. Then

$$\mathbb{E}(\mathrm{Gut}(T)) = 4\mathbb{E}(W(T)) - (2n-1)(n-1) \tag{1.2}$$

and

$$\mathbb{V}ar(\mathrm{Gut}(T)) = 16\mathbb{V}ar(W(T)). \tag{1.3}$$

Our aim in this paper is to consider the expected value and variance of the Gutman index and degree distance in random trees.

2. The Main Results

Let the generalized harmonic number for nonnegative n, complex order m and complex offset c be defined as:

$$H_{c,n}^{(m)} = \sum_{k=1}^{n} \frac{1}{(c+k)^m}.$$

For ease of notation the following convention is used:

$$H_n^{(m)} = H_{0,n}^{(m)}.$$

The traditional harmonic numbers are a special case:

$$H_n = H_n^{(1)}.$$

We have

$$\sum_{k=1}^{n} H_k = (n+1)H_{n+1} - (n+1), \tag{2.1}$$

$$\sum_{k=1}^{n} H_k^{(2)} = (n+1)H_{n+1}^{(2)} - H_{n+1}, , \tag{2.2}$$

$$\sum_{k=1}^{n} \frac{H_k}{k} = \frac{1}{2}(H_n^2 + H_n^{(2)}), \tag{2.3}$$

$$\sum_{k=1}^{n} kH_k = \frac{n(n+1)}{2}H_{n+1} - \frac{n(n+1)}{4}, \tag{2.4}$$

$$\sum_{k=1}^{n} kH_k^{(2)} = \frac{n(n+1)}{2}H_{n+1}^{(2)} + \frac{1}{2}H_{n+1} - \frac{n+1}{2}. \tag{2.5}$$

In the discourse we shall use the following notations:

$$\begin{aligned}
&T_{i,v,c} = vH_i - cH_i^{(2)}, \ i \geq 1, c, v \in \mathbb{R} \\
&L_{i,m,n} = \frac{i(i-1)}{2}T_{i-1,1,m} + \frac{i(i+1)}{2}T_{i+1,1,n}, \\
&D_i = i(i-1)T_{i,1,2} + i(i+1)T_{i+2,1,6}, \\
&V_i = (i+1)(2T_{i+2,1,6} + T_{i+1,66,60}), \\
&P_i = \sum_{k=1}^{i} H_k^2, \\
&a(n;a,b,c,d) = \frac{an^2+bn+c}{2d}, \ n \geq 1.
\end{aligned}$$

Kuba and Panholzer [19] gave a distributional analysis of the random variable $d(j,n)$, which counts the distance, measured by the number of edges lying on the connecting path, between node j and node n in a random tree of order n. They showed that the expectation of the random variable $d(j,n)$

(for $1 \leq j < n$) are given by

$$\begin{aligned} &1)\ \mathbb{E}(d_{RT}(j,n)) = H_{n-1} + H_j + \frac{1}{j} - 2,\\ &2)\ \mathbb{E}(d_{BIT}(j,n)) = 2H_n + 2H_{j+1} + \frac{6}{j+1} - 8,\\ &3)\ \mathbb{E}(d_{PORT}(j,n)) = H_{2n-2} - \frac{1}{2}H_{n-1} + H_{2j} - \frac{1}{2}H_j - 1. \end{aligned} \tag{2.6}$$

Also, they showed that for the variances:

$$\begin{aligned} &1)\mathbb{V}ar(d_{RT}(j,n)) = \mathbb{E}(d_{RT}(j,n)) - H_{n-1}^{(2)} - 3H_j^{(2)} - \frac{4}{j}H_j + 6 + \frac{2}{j} - \frac{1}{j^2},\\ &2)\mathbb{V}ar(d_{BIT}(j,n)) = \mathbb{E}(d_{BIT}(j,n)) - 4H_n^{(2)} - 12H_{j+1}^{(2)} - \frac{48}{j+1}H_{j+1} + 34\\ &+\frac{60}{j+1} - \frac{36}{(j+1)^2},\\ &3)\mathbb{V}ar(d_{PORT}(j,n)) = \mathbb{E}(d_{PORT}(j,n)) - H_{2n-2}^{(2)} + \frac{1}{4}H_{n-1}^{(2)} - 3H_{2j}^{(2)} + \frac{3}{4}H_j^{(2)} + 3. \end{aligned} \tag{2.7}$$

Let W_n^{RT} be the Wiener index of a random recursive tree T of order n. Neininger [21] showed that for random recursive trees,

$$\mathbb{E}(W_n^{RT}) = n^2H_n + nH_n - 2n^2.$$

He used the recursive structure of the tree in order to setup a recurrence for the Wiener index. He decomposed the tree into the subtree rooted at the vertex labelled 2 and the rest of the tree, which is then rooted at the root of the original tree. He obtained by enumeration

$$W_n^{RT} \overset{D}{=} W_{I_n}^{RT} + W_{J_n}^{\prime RT} + J_nP_{I_n} + I_nP'_{J_n} + I_nJ_n,$$

where the cardinality I_n of the subtree rooted at the vertex labelled 2 is uniformly distributed on $\{1,\ldots,n-1\}$ for $n \geq 2$ and that conditioned on its cardinality this subtree and the rest of the tree are random recursive trees of cardinalities I_n and $J_n := n - I_n$, respectively being independent of each other. Also, (W_n^{RT}, P_n) and $(W_n^{\prime RT}, P'_n)$ are the pairs of the Wiener index and the internal path lengths in random recursive trees.

In this paper, we use another recurrence for the Wiener index of random recursive trees and obtain the above result. Also, we extend this approach to the analysis of the degree distance and Gutman index in increasing trees. Also, we give the lower and upper bounds for the variance of these quantities.

Theorem 2.1. *Let G_n be the Gutman index of an increasing tree of order n. Then*
1) for recursive trees,

$$\mathbb{E}(G_n^{RT}) = 4(n^2+n)H_n - 10n^2 + 3n - 1,$$

2) for binary increasing trees,

$$\mathbb{E}(G_n^{BIT}) = (8n^2 + 32n + 24)H_{n+1} - 26n^2 + 51n - 25,$$

3) for plane-oriented recursive trees,

$$\mathbb{E}(G_n^{PORT}) = 4E_{n-1} + 2nH_n + 4\sum_{k=1}^{n-1} F_{k,1} - 3n^2 + 2n - 1,$$

where $E_m := \sum_{j=1}^{m} jH_{2j}$ *and* $F_{m,a} := \sum_{j=1}^{m} H_{2j}^{(a)}$.

Proof. Let W_n be the Wiener index of an increasing tree of order n. By definition of the Wiener index and stochastic growth rule of the tree,

$$W_n = W_{n-1} + \sum_{j=1}^{n-1} d_T(j,n), \tag{2.8}$$

where $d_T(j,n)$ is the distance between node labelled $j \leq n-1$ and node n of T.

1) From (2.6), part (1) and (2.1),

$$\begin{aligned}
\mathbb{E}(W_n^{RT}) &= \mathbb{E}(W_{n-1}^{RT}) + \sum_{j=1}^{n-1} \mathbb{E}(d_{RT}(j,n)) \\
&= \mathbb{E}(W_{n-1}^{RT}) + \sum_{j=1}^{n-1} (H_{n-1} + H_j + j^{-1} - 2) \\
&= \mathbb{E}(W_{n-1}^{RT}) + nH_{n-1} + \sum_{j=1}^{n-1} H_j - 2(n-1) \\
&= \mathbb{E}(W_{n-1}^{RT}) + n(H_n + H_{n-1}) - 3n + 2, \qquad (2.9)
\end{aligned}$$

where $W_1^{RT} = 0$. Thus, the recurrence equation (2.9) leads to

$$\mathbb{E}(W_n^{RT}) = \sum_{k=1}^{n} k\Big(2H_k - \frac{1}{k}\Big) - 3\frac{n(n+1)}{2} + 2n. \tag{2.10}$$

From (2.4),

$$\begin{aligned}
\mathbb{E}(W_n^{RT}) &= 2\Big(\frac{n(n+1)}{2} H_{n+1} - \frac{n(n+1)}{4}\Big) - n - 3\frac{n(n+1)}{2} + 2n \\
&= n(n+1)\Big(H_n + \frac{1}{n+1}\Big) - 2n(n+1) - n + 2n \\
&= n^2 H_n + nH_n - 2n^2.
\end{aligned}$$

Now, from (1.2), $\mathbb{E}(G_n^{RT}) = 4(n^2+n)H_n - 10n^2 + 3n - 1$.

2) With the same manner and using (2.6), part (2),

$$\mathbb{E}(W_n^{BIT}) = \mathbb{E}(W_{n-1}^{BIT}) + 4nH_n + 6H_n - 10n.$$

Then

$$\mathbb{E}(W_n^{BIT}) = (2n^2 + 8n + 6)H_{n+1} - 6(n^2 + 2n + 1).$$

3) We have

$$(n-1)H_{n-1} - nH_n = 1 - H_{n-1}. \tag{2.11}$$

From (2.1) and (2.11),

$$\begin{aligned}\mathbb{E}(W_n^{PORT}) &= \mathbb{E}(W_{n-1}^{PORT}) + \sum_{j=1}^{n-1} \mathbb{E}(d_{PORT}(j,n)) \\ &= \mathbb{E}(W_{n-1}^{PORT}) + \sum_{j=1}^{n-1} (H_{2n-2} - \frac{1}{2}H_{n-1} + H_{2j} - \frac{1}{2}H_j - 1) \\ &= \mathbb{E}(W_{n-1}^{PORT}) + (n-1)H_{2n-2} + \frac{1}{2}(H_{n-1}+1) - \frac{n}{2} + \sum_{j=1}^{n-1} H_{2j}. \qquad (2.12)\end{aligned}$$

Now, the recurrence equation (2.12) leads to

$$\mathbb{E}(W_n^{PORT}) = E_{n-1} + \frac{n}{2}\Big(H_n - \frac{n+1}{2}\Big) + \sum_{k=1}^{n-1} F_{k,1}$$

and proof is completed. □

Definition 2.2. *The degree distance of G is defined as* [22]

$$DD(G) = \sum_{\{u,v\}\subseteq V(G)} (d(u)+d(v))d_G(u,v).$$

The relations between the degree distance and the Wiener index was studied in [3, 9]. An example of such relation,

$$DD(T) = 4W(T) - n(n-1).$$

Theorem 2.3. *Let S_n be the degree distance of an increasing tree of order n. Then*
1) for recursive trees,

$$\mathbb{E}(S_n^{RT}) = 4(n^2+n)H_n - 9n^2 + 1,$$

2) for binary increasing trees,

$$\mathbb{E}(S_n^{BIT}) = (8n^2+32n+24)H_{n+1} - 25n^2 + 50n - 24,$$

3) for plane-oriented recursive trees,

$$\mathbb{E}(S_n^{PORT}) = 4E_{n-1} + 2nH_n + 4\sum_{k=1}^{n-1} F_{k,1} - 2n^2.$$

In passing, we give the lower and upper bounds for the variance of G_n and S_n.

Theorem 2.4. *For an increasing tree of order n (=RT, BIT and PORT),*

$$\mathbb{V}ar(S_n) = \mathbb{V}ar(G_n) \leq \Big(\frac{(n-1)(2n^2-10n+12)}{6}\Big)^2.$$

Proof. It is an immediate consequence of inequality (1.1) and Popoviciu's inequality. □

Theorem 2.5. *For an increasing tree of order n,*

$$\mathbb{V}ar(G_n) = \mathbb{V}ar(S_n) \geq 16 \max\{0, Q_n\},$$

where

1) for recursive trees,

$$Q_n = L_{n,1,3} + 3\Big(n + \frac{1}{2}\Big)H_{n+1} + H_n - 2P_{n-1} + 3nT_{n,1} + a(n; 5, -29, -6, 2),$$

2) for binary increasing trees,

$$Q_n = D_n + V_n + 60H_{n+1} + 6(2n+3)H_{n+2} - 24P_n + a(n; 23, -123, -25, 1),$$

3) for plane-oriented recursive trees,

$$Q_n = \frac{n(n-1)}{2}T_{2n-2,1,1} - 2L_{n+1,1/2,3/2} - \frac{3}{8}(2n+1)H_{n+1} + \sum_{k=1}^{n-1}(F_{k,1} - F_{k,2}) + a(n; 11, 1, 6, 4).$$

Proof. From (2.8),

$$W_n = \sum_{k=1}^{n-1}\sum_{j=1}^{k} d_T(j,n).$$

Thus

$$\begin{aligned}
\mathbb{V}ar(W_n^{RT}) &= \mathbb{V}ar\Big(\sum_{k=1}^{n-1}\sum_{j=1}^{k} d_{RT}(j,n)\Big)\\
&\geq \sum_{k=1}^{n-1}\sum_{j=1}^{k} \mathbb{V}ar(d_{RT}(j,n))\\
&= \sum_{k=1}^{n-1}(kH_{n-1} + (k+1)H_{k+1} - (k+1) - kH_{n-1}^{(2)} - 3\sum_{j=1}^{k} H_j^{(2)}\\
&- 4\sum_{j=1}^{k} j^{-1}H_j + 4k + 3H_k - H_k^{(2)}).
\end{aligned}$$

From (2.2), (2.3) and (2.5) and simplification,

$$\mathbb{V}ar(W_n^{RT}) = L_{n,1,3} + 3\Big(n + \frac{1}{2}\Big)H_{n+1} + H_n - 2P_{n-1} + 3nT_{n,1} + a_n.$$

With the same manner, we can obtain another bounds. □

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