ON THE WIENER INDEX OF TREES FROM CERTAIN FAMILIES

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ABSTRACT. The Wiener index $W(G)$ of a connected graph G is the sum of the distances between all pairs of vertices of G. We determine the expected value of $W(T_n)$ for trees T_n from certain families.

1. Introduction

The *Wiener index* $W(G)$ of a connected graph G is the sum of the distances $d(u, v)$ between all pairs of vertices u and v of G. This index seems to have been introduced in [22] where it was shown that certain physical properties of various paraffin species are correlated with the Wiener index of the tree determined by the carbon atoms of the corresponding molecules. Canfield, Robinson, and Rouvray [1] described a recursive procedure for determining the Wiener index of a tree and gave an extensive list of papers involving chemical applications of the index; see also [18] for an expository account of work in this area. More recently, McKay, and also Merris (see e.g. [10], [11], or [14]), have

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shown that the Wiener index $W(T_n)$ of a tree T_n has a simple expression in terms of the positive eigenvalues of a matrix associated with T_n. Additional material involving distances in trees may be found in [12], [13], and [23]. We remark that Plesnik [15] has given a general survey of results on sums of distances in graphs and digraphs.

If T_n is any tree with n vertices, then

$$(n-1)^2 \leq W(T_n) \leq \tfrac{1}{6}\, n(n^2-1)$$

with equality holding if and only if T_n is a star or a path, respectively [2]. Our object here is to consider the expected value of $W(T_n)$ over all trees T_n in certain families of trees. In §2 we describe the families we shall be considering — the simply generated families of trees. Our main results are in §3 where we show that under certain assumptions the expected value of $W(T_n)$ is asymptotic to $Qn^{5/2}$ as $n \to \infty$ for the families we are considering, where the value of the constant Q depends on the particular family involved. In §4 we illustrate these results in some special cases where explicit formulas can be obtained.

2. Simply Generated Families

We recall that *ordered* trees are rooted trees with an ordering specified for the branches incident with each vertex as one proceeds away from the root (see [6; p. 306]). Let $\mathcal{F}$ denote a family of weighted ordered trees in which the tree T_n has weight $c(T_n)$. Such a family is said to be *simply generated* (see, e.g. [9], [3], or [20]) if there exists a sequence of non-negative constants c_0 $(=1)$, $c_1, c_2, \ldots$ such that

$$c(T_n) = \Pi c_i^{N_i(T_n)} \tag{2.1}$$

for all trees T_n in $\mathcal{F}$, where $N_i(T_n)$ denotes the number of vertices of out-degree i in T_n. Let y_n denote the number of trees T_n in such a family $\mathcal{F}$ where (here and elsewhere) the weights are taken into account; that is

$$y_n = \sum c(T_n) \tag{2.2}$$

where the sum is over all ordered trees T_n with n vertices. It is not difficult to see (cf. [9], [3], or [20]) that the generating function $Y = \sum y_n x^n$ of such a simply generated family satisfies the relation

$$Y = x\Phi(Y) \tag{2.3}$$

where $\Phi(t) = 1 + \sum_1^\infty c_k t^k$. Three familiar examples of simply generated families are the ordinary ordered trees for which $\Phi(t) = (1-t)^{-1}$, the rooted labelled trees for which $\Phi(t) = e^t$, and the binary trees for which $\Phi(t) = 1 + t^2$. We remark, for later use, that the relation $Y = x\Phi(Y)$ implies that

$$xY' = Y \cdot \left(1 - x\Phi'(Y)\right)^{-1} \tag{2.4}$$

and that

$$x^2 Y'' = (xY'/Y) \cdot \{x\Phi''(Y) \cdot (xY')^2 + 2(xY' - Y)\}. \tag{2.5}$$

We shall assume henceforth that $\mathcal{F}$ is some particular simply generated family of trees whose generating function satisfies relation (2.3). And when deriving results of a general asymptotic nature, we shall assume the conditions of the following result hold (see [9; p. 999], [3; p. 203], or [20; p. 32]).

Lemma 1. *Suppose* $\Phi(t) = 1 + \sum_1^\infty c_k t^k$ *is an analytic function of* t *for* $|t| < R \le \infty$, *and let* $Y(x) = \sum_1^\infty y_n x^n$ *denote the unique solution of* $Y(x) = x\Phi(Y(x))$ *in the neighbourhood of* $x = 0$. *If*

(i) $c_k \ge 0$ *for* $k \ge 1$,
(ii) $gcd\{k : c_k > 0\} = 1$, *and*
(iii) $\tau\Phi'(\tau) = \Phi(\tau)$ *for some* τ, *where* $0 < \tau < R$, *then*

$$y_n \sim a\rho^{-n} n^{-3/2} \tag{2.6}$$

as $n \to \infty$, *where* $\rho = \tau/\Phi(\tau)$ *and* $a = \left(\Phi(\tau)/2\pi\Phi''(\tau)\right)^{1/2}$.

We shall also need the following asymptotic result; we omit the straightforward proof which involves approximating a sum by an integral.

Lemma 2. *Let* $P(x) = \sum_0^\infty p_n x^n$, $Q(x) = \sum_0^\infty q_n x^n$, *and* $P(x)Q(x) = \sum_0^\infty r_n x^n$, *and suppose there exist constants* $p, q, \rho > 0$ *and* $\alpha, \beta > -1$ *such that*

$$p_n \sim p\rho^{-n} n^\alpha \quad \text{and} \quad q_n \sim q\rho^{-n} n^\beta$$

as $n \to \infty$. *Then*

$$r_n \sim B(\alpha+1, \beta+1) \cdot pq\rho^{-n} n^{\alpha+\beta+1}$$

as $n \to \infty$, *where* $B(\alpha+1, \beta+1) = \int_0^1 t^\alpha (1-t)^\beta \, dt$ *is the beta function.*

3. Main Results

For any rooted tree T_n let $D(T_n)$ denote the sum of the distances $d(r,u)$ between the root-vertex r of T_n and the remaining $n-1$ vertices of T_n; and, as before, let $W(T_n)$ denote the sum of the distances $d(u,v)$ between the $n(n-1)/2$ pairs of distinct vertices u and v of T_n. (If $n=1$ then $D(T_n) = W(T_n) = 0$, by definition.) Let

$$d_n = \sum c(T_n) \cdot D(T_n) \quad \text{and} \quad w_n = \sum c(T_n) \cdot W(T_n)$$

where the sums are over all n-vertex trees T_n that belong to a particular simply generated family $\mathcal{F}$ and where $c(T_n)$ denotes the weight function defined in (2.1). We now derive relations for the generating functions

$$D(x) = \sum_1^\infty d_n x^n \quad \text{and} \quad W(x) = \sum_1^\infty w_n x^n.$$

(We remark that the general relation for $D(x)$ was derived in [9] and used to investigate the asymptotic behaviour of d_n; but it will be convenient to rederive the relation here by a somewhat different approach.)

Theorem. *Let* $F(x) = xY'(x)/Y(x) - 1$. *Then*

$$D(x) = xY'F \tag{3.1}$$

and

$$W(x) = x^2 Y' F'. \tag{3.2}$$

Proof. If we remove the root r of a non-trivial tree T_n in $\mathcal{F}$, along with all edges incident with r, we obtain a collection of disjoint rooted subtrees, or *branches*, $T^{(1)}, \ldots, T^{(k)}$ whose roots were originally joined to r. It follows readily from the relevant definitions that

$$D(T_n) = \sum_1^k D(T^{(i)}) + n - 1.$$

It is not difficult to see, bearing in mind the definition of simply generated families of trees, that this recursive relation for $D(T_n)$ implies that the generating function $D(x)$ satisfies the relation

$$
\begin{aligned}
D(x) &= x\sum_{1}^{\infty} c_k k Y^{k-1}(x)\cdot D(x) + xY'(x) - Y(x) \\
&= x\Phi'(Y)\cdot D(x) + xY'(x) - Y(x).
\end{aligned}
\tag{3.3}
$$

Conclusion (3.1) now follows upon solving for $D(x)$ and appealing to (2.4) and the definition of F.

We now consider the generating function $W(x)$. We assume, as before, that the non-trivial tree T_n is formed by joining the root-vertex r to the roots of the branches $T^{(1)},\ldots,T^{(k)}$. Now

$$W(T_n) = \sum d(u,v) = \Sigma_1 + \Sigma_2 + \Sigma_3$$

where $\Sigma_1, \Sigma_2,$ and Σ_3 denote the sum of the distances $d(u,v)$ between pairs of vertices u and v such that 1) one of the vertices u or v is the root-vertex r; 2) u and v belong to the *same* branch $T^{(i)}$ of T_n, where $1 \le i \le k$; and 3) u and v belong to *different* branches $T^{(i)}$ and $T^{(j)}$, where $1 \le i,\ j \le k$, respectively. It is not difficult to see that

$$\Sigma_1 + \Sigma_2 = D(T_n) + \sum_{1}^{k} W(T^{(i)}).$$

To obtain an expression for Σ_3 we observe that if r_i and r_j denote the roots of the distinct branches $T^{(i)}$ and $T^{(j)}$ containing vertices u and v, then

$$d(u,v) = \big(d(u,r_i)+1\big) + \big(d(v,r_j)+1\big).$$

From this it follows readily that the contribution to Σ_3 of all vertices in the i-th branch $T^{(i)}$ is equal to

$$\{D(T^{(i)}) + |T^{(i)}|\}\cdot \sum_{j\neq i} |T^{(j)}|,$$

where $|T^{(h)}|$ denotes the number of vertices in the branch $T^{(h)}$. Consequently,

$$
(3.4) \qquad \begin{aligned} W(T_n) &= \Sigma_1 + \Sigma_2 + \Sigma_3 \\ &= D(T_n) + \sum_{1}^{k} W(T^{(i)}) + \sum_{i \neq j} \{D(T^{(i)}) + |T^{(i)}|\} \cdot |T^{(j)}|, \end{aligned}
$$

where the last sum is over the $k(k-1)$ ordered pairs of distinct integers i and j such that $1 \leq i, j \leq k$. (We remark that this expression for $W(T_n)$ is equivalent to an expression given in [1; eq. (22)].)

It is not difficult to see that relation (3.4) implies that the generating function $W(x)$ satisfies the relation

$$
(3.5) \qquad W(x) = D(x) + x\Phi'(Y) \cdot W(x) + x\Phi''(Y) \cdot \{D(x) + xY'\} \cdot xY'.
$$

Now $D(x) + xY' = (xY')^2/Y$, by (3.1); and (2.5), (3.1), and the relation $xY' = YF + Y$ imply that

$$
(3.6) \qquad x\Phi''(Y) \cdot (xY')^3/Y = x^2Y'' - 2D = xYF' - D.
$$

Taking (2.4) into consideration, relation (3.2) now follows from (3.5) and (3.6).

We now determine the asymptotic behaviour of d_n and w_n over the y_n trees T_n in $\mathcal{F}$. We remind the reader that we are assuming the conditions of Lemma 1 hold so that $y_n \sim a\rho^{-n}n^{-3/2}$ where $\rho = \tau/\Phi(\tau)$ and $a = (\Phi(\tau)/2\pi\Phi''(\tau))^{1/2}$. In what follows we let $C_n\{g(x)\}$ denote the coefficient of x^n in the power series expansion of $g(x)$.

Corollary. *Let* $K = \pi a \tau^{-1}$; *then*

$$
(3.7) \qquad d_n \sim K n^{3/2} y_n
$$

and

$$
(3.8) \qquad w_n \sim \tfrac{1}{2} K n^{5/2} y_n,
$$

as $n \to \infty$.

Proof. We recall (see [8; p. 164]) that

$$
C_n\{F\} = C_n\{xY'/Y - 1\} \sim \tau^{-1} n y_n \sim \tau^{-1} a \rho^{-n} n^{-1/2}.
$$

It was shown in [9; p. 1005] that this, relation (3.1), and the case $\alpha = \beta = -1/2$ of Lemma 2 imply that

$$d_n \sim C_n\{xY'F\} \sim \pi\tau^{-1}a^2\rho^{-n} \sim Kn^{3/2}y_n$$

as $n \to \infty$. Furthermore, when we apply the case $\alpha = -1/2$ and $\beta = +1/2$ of Lemma 2 to relation (3.2) we find that

$$w_n = C_n\{xY' \cdot xF'\} \sim \tfrac{1}{2}\pi\tau^{-1}a^2\rho^{-n}n \sim \tfrac{1}{2}Kn^{5/2}y_n$$

as $n \to \infty$. This completes the proof of relations (3.7) and (3.8).

We remark that it can be shown, using (3.1) and (3.2), that

$$W = \tfrac{1}{2}xD' + \tfrac{1}{2}x^2Y'' - \tfrac{1}{2}FD - D$$

from which the conclusion $w_n \sim \frac{1}{2}\, nd_n \sim \frac{1}{2}\, Kn^{5/2}y_n$ can also be readily deduced by showing that $\frac{1}{2}\, xD'$ is the dominant term on the right-hand side. The relation $w_n \sim \frac{1}{2}\, nd_n$ implies that the average distance between the root-vertex of a tree T_n and the remaining $n-1$ vertices of T_n is asymptotically equal to the average distance between all the $n(n-1)/2$ pairs of vertices of T_n, where the averages are taken over all appropriate pairs of vertices in all the y_n trees T_n in $\mathcal{F}$.

4. Special Cases

We now illustrate the preceding results for some particular families of trees. Let $\mathcal{F}$ denote the family of ordinary ordered trees whose generating function Y satisfies the relation $Y = x(1-Y)^{-1}$. Then (see, e.g., [4; p. 112] or [20; p. 30])

$$Y = \tfrac{1}{2}\{1-(1-4x)^{1/2}\} = \sum_{1}^{\infty} \binom{2n-2}{n-1} \frac{x^n}{n}$$

and $Y' = (1-2Y)^{-1} = (1-4x)^{-1/2}$, so

$$F = xY'/Y - 1 = (1-Y)/(1-2Y) - 1 = \tfrac{1}{2}\{(1-2Y)^{-1} - 1\} = \tfrac{1}{2}(Y'-1). \tag{4.1}$$

In this case relation (3.1) implies that

$$\begin{aligned} D = xY'F &= \tfrac{1}{2}\, xY'(Y'-1) \\ &= \tfrac{1}{2}\, x\{(1-4x)^{-1} - (1-4x)^{-1/2}\}. \end{aligned}$$

Consequently,

$$d_n = 2^{2n-3} - \tfrac{1}{2} \binom{2n-2}{n-1} ,$$

a result given earlier in [21] and [9]. Furthermore, it follows from (3.2) and (4.1) that

$$W = x^2 Y' F' = \tfrac{1}{2}\, x^2 Y' Y'' = x^2 (1-4x)^{-2}.$$

Therefore

$$w_n = (n-1)4^{n-2} \tag{4.2}$$

and

$$w_n / y_n = n(n-1)4^{n-2} \Big/ \binom{2n-2}{n-1} \sim \tfrac{1}{4} \sqrt{\pi}\, n^{5/2}$$

as $n \to \infty$.

It is possible to give a more direct combinatorial proof of formula (4.2). First, select a pair of rooted ordered trees T_a and T_b where $a+b=n$; choose a pair of vertices u and v, one from each of the trees T_a and T_b; and then join the roots of T_a and T_b by an edge e. This can be done in $ay_a \cdot by_b$ ways, for given values of a and b. The tree T_n thus formed can be regarded as an unrooted tree embedded in the plane (with two designated vertices u and v separated by the designated edge e). Now choose one of the edges rs of T_n and then choose one of the two vertices joined by this edge — r, say; this can be done in $2(n-1)$ ways. If we regard r as the root-vertex of T_n and edge rs as the "first" or "left-most" edge incident with r, then this has the effect of inducing an ordering upon the edges incident with each vertex encountered in proceeding away from the root and, hence, of converting T_n into a rooted ordered tree (with two designated vertices u and v separated by a designated edge e). If we count the total number of ways of carrying out this construction, bearing in mind the symmetry between the two subtrees T_a and T_b, then it is not difficult to see that each rooted ordered tree T_n is counted separately for each edge e separating each pair of vertices u and v in T_n; that is, each such tree T_n is counted $W(T_n)$ times. Therefore,

$$\begin{aligned}
w_n &= 2(n-1)\cdot\tfrac{1}{2}\sum_{1}^{n-1} a y_a \cdot (n-a) y_{n-a} \\
&= (n-1)\cdot \mathcal{C}_n\{(xY')^2\} \\
&= (n-1)\cdot \mathcal{C}_n\{x^2(1-4x)^{-2}\} = (n-1)\cdot 4^{n-2},
\end{aligned} \tag{4.3}$$

as required. We remark that the basic observation on which the foregoing argument relies, namely, that $W(T_n)$ equals the sum, over all edges e of the tree T_n, of the number of pairs of vertices separated by e, appears in [22; p. 17, par. 4].

We turn from simply generated trees for a moment to point out that formula (4.2) for the sum $\sum W(T_n)$ over all ordered trees gives rise to a corresponding formula for a closely related family of trees. Labelled plane trees may be defined as the equivalence classes of trees with labelled vertices embedded in the plane under orientation-preserving homeomorphisms of the plane to itself. Let L_n denote the number of these trees with n vertices, and let y_n still denote the number of rooted ordered trees T_n. We can convert any labelled plane tree with $n \geq 2$ vertices into a rooted ordered tree T_n with labelled vertices in $2(n-1)$ ways by, as before, selecting an incident vertex and edge — r and rs, say — to serve as the root-vertex and as the "first" or "left-most" edge incident with the root. On the other hand, the number of ways of assigning the labels $1, 2, \ldots, n$ to the vertices of a rooted ordered tree T_n is clearly $n!$ (see [6; p. 586, exer. 23]). Consequently

$$2(n-1)L_n = n!\, y_n,$$

and

$$\begin{aligned}
L_n &= \frac{n!}{2(n-1)} \cdot \binom{2n-2}{n-1}\frac{1}{n} \\
&= (2n-3)_{n-2}
\end{aligned}$$

for $n \geq 2$. This correspondence between labelled plane trees and ordered trees preserves distances between vertices; so it follows from (4.2) that the sum $\sum W(T_n)$ over the L_n labelled plane trees with n vertices equals

$$\frac{n!}{2(n-1)} \cdot (n-1)4^{n-2} \quad \text{or} \quad n! \cdot 2^{2n-5}$$

for $n \geq 2$.

Now let $\mathcal{F}$ denote the family of rooted labelled trees whose generating function Y satisfies the relation $Y = xe^Y$. Then (see [4; p. 174] or [6; p. 392])

(4.4)
$$Y = \sum_1^\infty n^{n-1} \frac{x^n}{n!}$$

and $xY' = Y(1-Y)^{-1}$, so

(4.5)
$$F = xY'/Y - 1 = (1-Y)^{-1} - 1 = Y(1-Y)^{-1} = xY'.$$

In this case relation (3.1) implies that

(4.6)
$$D = xY'F = (xY')^2,$$

a result given earlier in [17] and [9; p. 1006]. Consequently,

(4.7)
$$d_n/y_n = n^{1-n} \cdot \sum_1^{n-1} \binom{n}{k} k^k (n-k)^{n-k},$$

in view of (4.4) and (4.6). Riordan and Sloane [17; p. 281] pointed out that

$$\sum_1^{n-1} \binom{n}{k} k^k (n-k)^{n-k} = n^n \cdot \sum_2^n (n)_k / n^k,$$

by the Cauchy formula [16; p. 21] associated with Abel's generalization of the binomial theorem. Knuth [6; p. 117] has investigated the asymptotic behaviour of this last sum and shown that the dominant term is $(\pi n/2)^{1/2}$. (Another way to reach this conclusion is to rewrite the sum as

$$n! \cdot (e/n)^n \cdot \sum_0^{n-2} e^{-n} n^j / j!$$

and then appeal to Stirling's formula and the normal approximation to the Poisson distribution; cf. [5; p. 515] or [19; p. 619].) Hence

(4.8)
$$d_n/y_n = n \sum_2^n (n)_k / n^k \sim \sqrt{\pi/2}\, n^{3/2}$$

as $n \to \infty$, a result appearing in [17] and [9].

It follows from (3.2), (4.5), and (4.6) that

$$W = x^2Y'F' = x(xY')\cdot(xY')' = \tfrac{1}{2}\,x\,\frac{d}{dx}\,(xY')^2 = \tfrac{1}{2}\,xD'.$$

Therefore,

$$w_n = \tfrac{1}{2}\,nd_n$$

and

$$w_n/y_n = \tfrac{1}{2}\,n\cdot n^{1-n}\cdot\sum_{1}^{n-1}\binom{n}{k}\,k^k(n-k)^{n-k} \tag{4.9}$$
$$= \tfrac{1}{2}\,n^2\cdot\sum_{2}^{n}(n)_k/n^k \sim \sqrt{\pi/8}\,n^{5/2}$$

as $n\to\infty$, by (4.7) and (4.8).

We remark that the relation $w_n = \tfrac{1}{2}\,nd_n$ is obvious for the family of rooted labelled trees. Also, the argument used to establish formula (4.3) can be adapted to provide a direct combinatorial derivation of the first expression for w_n/y_n in (4.9). The main difference is that we must allow for the fact that the vertices are labelled now; and, instead of the factor $2(n-1)$ we now have simply the factor n to account for the number of ways of selecting the root-vertex.

Finally, let $\mathcal{F}$ denote the family of rooted binary trees whose generating function Y satisfies the relation $Y = x(1+Y^2)$. Then (see [20; p. 29] or [6; p. 389])

$$Y = (2x)^{-1}\cdot\{1-(1-4x^2)^{1/2}\} = \sum_{1}^{\infty}\binom{2n-2}{n-1}\frac{x^{2n-1}}{n}$$

and $xY'/Y = (1-2xY)^{-1} = (1-4x^2)^{-1/2}$, so

$$F = xY'/Y - 1 = (1-2xY)^{-1} - 1 \tag{4.10}$$
$$= 2xY\cdot(1-2xY)^{-1} = 2x^2Y'.$$

In this case relation (3.1) implies that

$$D = xY'F = 2x(xY')^2 \tag{4.11}$$
$$= (2x)^{-1}\cdot\{1+(1-4x^2)^{-1} - 2(1-4x^2)^{-1/2}\},$$

so

$$d_{2n-1} = 2^{2n-1} - \binom{2n}{n},$$

a result given earlier in [7; p. 590], in effect, and in [9; p. 1009]. Furthermore, it follows from (3.2), (4.10), and (4.11) that

$$W = x^2Y'F' = 2x^2Y' \cdot (x^2Y')' = \frac{d}{dx}\,(x^2Y')^2 = \tfrac{1}{2}\,(xD)'.$$

Therefore,

$$w_{2n-1} = nd_{2n-1} = n2^{2n-1} - n\,\binom{2n}{n}$$

and

$$w_{2n-1}/y_{2n-1} \sim 2\sqrt{\pi}\,n^{5/2}$$

as $n \to \infty$.

Notice that the relation $w_{2n-1} = nd_{2n-1}$ is equivalent to the relation $w_{2n-1} = 2nC_{2n-2}\{(xY')^2\}$, in view of (4.11). It is possible to give a combinatorial proof of this last relation by a modification of the argument used earlier to derive relation (4.3). This time, however, the rooting process involves inserting a new vertex in one of the edges; and we must take into account the effect this has on the distances between vertices separated by this new vertex. The details are not particularly complicated, but we shall not include them here.

We remark in closing that the constant K that appears in the corollary may assume any positive value for suitable families $\mathcal{F}$. For example, when $Y = x(1+\beta Y + \frac{1}{4}\gamma^2Y^2)$, where β and γ are positive constants, we find that $K = \left(\frac{1}{2}\pi(1+\beta/\gamma)\right)^{1/2}$; this takes on all values in the interval $(\sqrt{\pi/2}, \infty)$ as β varies throughout the inverval $(0,\infty)$. When $Y = x(1-\beta Y)^{-\gamma}$ we find that $K = \left(\pi\gamma/2(1+\gamma)\right)^{1/2}$ and this takes on all values in the interval $(0, \sqrt{\pi/2})$ as γ varies throughout the interval $(0,\infty)$. Finally, when $Y = xe^Y$ we find that $K = \sqrt{\pi/2}$.

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