On the General Randić Index for Certain Families of Trees

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Abstract. The general Randić index $w_\alpha(G)$ of a graph G is the sum of the weights $(d_G(u)d_G(v))^\alpha$ of all edges uv of G. We give bounds for $w_{-1}(T)$ when T is a tree of order n. We also show that $\lim_{n\to\infty} f(n)/n$ exists, and give bounds for the limit, where $f(n) = \max\{w_{-1}(T) \colon T$ is a tree of order $n\}$. Finally, we find the expected value and variance of w_α for certain families of trees.

I. Introduction

In studying branching properties of alkanes, Randić [7] proposed several numbering schemes for the edges of the associated hydrogen-suppressed graph based on the degrees of the end vertices of an edge. To preserve rankings of certain molecules, several inequalities involving the weights of edges needed to be satisfied (only the seven inequalities arising from the isomers of the smaller members butane, pentane and hexane were required). Randić [7, p. 6611] stated that weighting all edges uv of the associated graph G by $(d_G(u)d_G(v))^{-1}$ or all by $(d_G(u)d_G(v))^{-1/2}$ preserved these inequalities and eventually chose the latter. The sum of these latter weights over the edges of G – sometimes called the Randić index of G – has been closely correlated with many chemical properties (see [4]). We are interested in the former index proposed by Randić, and extensions, for trees. First, we provide a general setting and a survey of some known results.

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Fix $\alpha \in \mathbb{R} - \{0\}$. For an edge uv of a graph G, let $w_\alpha(uv) = (d_G(u)d_G(v))^\alpha$ and let $w_\alpha(G) = \sum_{uv \in E(G)} w_\alpha(uv)$ denote the **general Randić index** of G. Hence, $w_{-1/2}(G)$ is the ordinary Randić index of G. Yu [11] gave the sharp upper bound of $w_{-1/2}(T) \leq (n + 2\sqrt{2} - 3)/2$ when T is a tree of order n. Bollobás and Erdös [1] gave the sharp lower bound of $w_{-1/2}(G) \geq \sqrt{n-1}$ when G is a graph of order n without isolated vertices; a sharp upper bound for $w_\alpha(G)$, $\alpha \in (0, 1]$, when G is a graph of size m; and a sharp lower bound for $w_\alpha(G)$, $\alpha \in [-1, 0)$, when G is a graph of size m. In this paper we give several extremal and probabilistic results for $w_\alpha(T)$ for T belonging to certain families of trees.

The set of vertices (edges) of a simple graph G is denoted by $V(G)$ ($E(G)$). The order of G is $|V(G)|$. The degree $d_G(u)$ of a vertex u is the number of vertices in G which are adjacent to u. A vertex of degree one in a tree is called a leaf. The path of order n is denoted by P_n. The star $K_{1,m}$ in which each edge has been replaced with a path of length 2 is denoted by $K^*_{1,m}$. The nonnegative integers are denoted by $\mathbb{N}$ and the real numbers by $\mathbb{R}$. All notation, terminology and presumed results may be found in West [9].

II. Bounds for $\mathbf{w_{-1}(T)}$

We first give bounds for $w_{-1}(T)$ (see [1] for a related, but different, result). We assume the trees have vertex set $[n] := \{1, \ldots, n\}$.

Theorem 1. For a tree T of order $n \geq 2$,

$$1 \leq w_{-1}(T) \leq \frac{5n+8}{18}.$$

Proof. The lower bound follows immediately from (1) below, hence, we only consider the upper bound. By way of contradiction, let T be a tree of order n with $w_{-1}(T) > (5n+8)/18$ where n is as small as possible. We deduce a number of properties of T. Our result is readily seen to be true for all $2 \leq n \leq 8$, so $n \geq 9$. Since $1 = w_{-1}(K_{1,n-1}) \leq (5n+8)/18$ and $(m+1)/2 = w_{-1}(K^*_{1,m}) \leq (10m+13)/18$, $T \ncong K_{1,n-1}$ nor $K^*_{1,m}$. Let $x_1, \ldots, x_r$ ($r \geq 1$) be the leaves of T adjacent to a vertex y and $z_1, \ldots, z_s$ be the other vertices of T adjacent to y, where $r + s$ is as large as possible. Then $s \geq 1$ (as $T \ncong K_{1,n-1}$) and all $d_T(z_j) \geq 2$. Now ($2 \leq n - r \leq n - 1$),

$$w_{-1}(T) = w_{-1}(T - \{x_1, \ldots, x_r\}) - \frac{r}{s(r+s)} \sum_{j=1}^{s} \frac{1}{d_T(z_j)} + \frac{r}{r+s} \qquad (1)$$

$$\leq \frac{5(n-r)+8}{18} - \frac{r}{s(r+s)}\sum_{j=1}^{s}\frac{1}{d_T(z_j)} + \frac{r}{r+s} \leq \frac{5n+8}{18}, \qquad (2)$$

provided $r+s \geq 4$, hence, $r+s \leq 3$.

Suppose $r=2$ and $s=1$. Then (2) holds for $d_T(z_1) \leq 6$. Let $w_1, \ldots, w_t$ ($t \geq 6$) be the vertices of T, other than y, adjacent to z_1. Now ($n-3 \geq 7$),

$$w_{-1}(T) = w_{-1}(T - \{x_1, x_2, y\}) - \frac{1}{t(t+1)}\sum_{j=1}^{t}\frac{1}{d_T(w_j)} + \frac{1}{3(t+1)} + \frac{2}{3}$$
$$\leq \frac{5(n-3)+8}{18} + \frac{5}{7} < \frac{5n+8}{18}.$$

Suppose $r=1$ and $s=2$. Now ($n-2 \geq 7$),

$$w_{-1}(T) = w_{-1}(T + z_1z_2 - \{x_1, y\}) - \frac{1}{d_T(z_1)d_T(z_2)} + \frac{1}{3d_T(z_1)}$$
$$+ \frac{1}{3d_T(z_2)} + \frac{1}{3}$$
$$\leq \frac{5(n-2)+8}{18} - \frac{1}{d_T(z_1)d_T(z_2)} + \frac{1}{3d_T(z_1)} + \frac{1}{3d_T(z_2)} + \frac{1}{3}$$
$$\leq \frac{5n+8}{18}$$

provided

$$\frac{1}{3d_T(z_1)} + \frac{1}{3d_T(z_2)} \leq \frac{2}{9} + \frac{1}{d_T(z_1)d_T(z_2)}. \qquad (3)$$

Considering $d_T(z_1)$ and $d_T(z_2) \geq 3$; $d_T(z_1) = 2$ and $d_T(z_2) \geq 3$; $d_T(z_1) \geq 3$ and $d_T(z_2) = 2$; and $d_T(z_1) = d_T(z_2) = 2$ shows that (3) holds.

Hence, $r=s=1$. Then (2) holds for $d_T(z_1) = 2$. Let $w_1, \ldots, w_t$ ($t \geq 2$) be the vertices of T, other than y, adjacent to z_1. Now ($n-2 \geq 7$),

$$w_{-1}(T) = w_{-1}(T - \{x_1, y\}) - \frac{1}{t(t+1)}\sum_{j=1}^{t}\frac{1}{d_T(w_j)} + \frac{1}{2(t+1)} + \frac{1}{2}$$
$$\leq \frac{5(n-2)+8}{18} + \frac{1}{2(t+1)} + \frac{1}{2} \leq \frac{5n+8}{18},$$

provided $t \geq 8$. Hence, each leaf x in T is on a path x, y, z with $d_T(y) = 2$ and $d_T(z) = 3$, 4, 5, 6, 7 or 8 (as $r+s$ is as large as possible). We call x, y, z a **suspended path** from x to z. Let $x_1, \ldots, x_j$ ($j \geq 1$) be the distinct leaves of T on suspended paths $x_1, y_1, z; \cdots; x_j, y_j, z$ and $w_1, \ldots, w_{d-j}$ be the vertices of T, other than $y_1, \ldots, y_j$, adjacent to z (which we call a **(j, d)-system centered at z**). Hence, $1 \leq j \leq d-1 \leq 7$, $d \geq 3$ (as $T \not\cong K^*_{1,m}$). Now ($n-2 \geq 7$),

$$
\begin{aligned}
w_{-1}(T) &= w_{-1}(T - \{x_1, y_1\}) - \frac{1}{d(d-1)} \sum_{i=1}^{d-j} \frac{1}{d_T(w_i)} + \frac{d-j}{2d(d-1)} + \frac{1}{2} \\
&\leq \frac{5(n-2)+8}{18} - \frac{1}{d(d-1)} \sum_{i=1}^{d-j} \frac{1}{d_T(w_i)} + \frac{d-j}{2d(d-1)} + \frac{1}{2} \\
&\leq \frac{5n+8}{18}
\end{aligned}
$$

provided

$$
\frac{d-j}{2d(d-1)} \leq \frac{1}{18} + \frac{1}{d(d-1)} \sum_{i=1}^{d-j} \frac{1}{d_T(w_i)}. \tag{4}
$$

We examine (4) for all pairs (j, d) with $1 \leq j \leq d-1 \leq 7$, $d \geq 3$. Now $(d-j)/2d(d-1) \leq 1/18$ for $(j,d) = (3,4)$, $(3,5)$, $(4,5)$, $(3,6)$, $(4,6)$, $(5,6)$, $(3,7)$, $(4,7)$, $(5,7)$, $(6,7)$, $(2,8)$, $(3,8)$, $(4,8)$, $(5,8)$, $(6,8)$ or $(7,8)$, so (4) holds for these pairs. Also, (4) holds for $(j,d) = (1,3)$ unless some $d_T(w_i) \geq 4$; $(2,3)$ unless some $d_T(w_i) \geq 7$; $(1,4)$ unless some $d_T(w_i) \geq 4$; $(2,4)$ unless some $d_T(w_i) \geq 7$; $(1,5)$ unless some $d_T(w_i) \geq 5$; $(2,5)$ unless some $d_T(w_i) \geq 8$; $(1,6)$ unless some $d_T(w_i) \geq 7$; $(2,6)$ unless some $d_T(w_i) \geq 13$; $(1,7)$ unless some $d_T(w_i) \geq 10$; $(2,7)$ unless some $d_T(w_i) \geq 31$; and $(1,8)$ unless some $d_T(w_i) \geq 19$.

For each such (j,d)-system centered at z, take the edges of the j suspended paths along with the distinguished edge zw_i with $d_T(w_i)$ as specified above where, say, w_i is as small as possible (recall $V(T) = [n]$). By considering the degrees of both ends of the distinguished edge, it is easily seen that the collection of all such edge-sets is pair-wise disjoint except, possibly, that pairs of $(1,4)$-systems or pairs of $(1,5)$-systems share their distinguished edge. Let $m_{j,d}$ denote the number of such (j,d)-systems in T; $m^*_{1,4}$ denote the number of **pairs** of $(1,4)$-systems sharing their distinguished edge; and $m^*_{1,5}$ denote the number of **pairs** of $(1,5)$-systems sharing their distinguished edge. Then, when we calculate the weights of these specified edges belonging to these systems we find that,

$$
w_{-1}(T) \leq \frac{3}{4} m_{1,3} + \frac{29}{21} m_{2,3} + \frac{11}{16} (m_{1,4} - 2m^*_{1,4}) + \frac{21}{16} m^*_{1,4} + \frac{9}{7} m_{2,4}
$$

$$
\begin{aligned}
&+\frac{16}{25}(m_{1,5}-2m^*_{1,5})+\frac{31}{25}m^*_{1,5}+\frac{49}{40}m_{2,5}+\frac{17}{28}m_{1,6}+\frac{46}{39}m_{2,6}\\
&+\frac{41}{70}m_{1,7}+\frac{249}{217}m_{2,7}+\frac{173}{304}m_{1,8}+\frac{1}{4}\{n-1-3[m_{1,3}+\\
&\quad (m_{1,4}-2m^*_{1,4})+(m_{1,5}-2m^*_{1,5})+m_{1,6}+m_{1,7}+m_{1,8}]\\
&\quad -5[m^*_{1,4}+m^*_{1,5}+m_{2,3}+m_{2,4}+m_{2,5}+m_{2,6}+m_{2,7}]\}\\
=&\frac{n-1}{4}+\frac{11}{84}m_{2,3}-\frac{1}{16}m_{1,4}+\frac{3}{16}m^*_{1,4}+\frac{1}{28}m_{2,4}-\frac{11}{100}m_{1,5}\\
&+\frac{21}{100}m^*_{1,5}-\frac{1}{40}m_{2,5}-\frac{1}{7}m_{1,6}-\frac{11}{156}m_{2,6}-\frac{23}{140}m_{1,7}\\
&-\frac{89}{868}m_{2,7}-\frac{55}{304}m_{1,8}\\
\le&\frac{n-1}{4}+\frac{11}{84}m_{2,3}+\frac{1}{32}m_{1,4}+\frac{1}{28}m_{2,4},
\end{aligned}
$$

since each remaining non-specified edge has weight at most $1/4$ while $2m^*_{1,4} \le m_{1,4}$ and $2m^*_{1,5} \le m_{1,5}$. Now the maximum of $11x/84+y/32+z/28$ where x, y, z are nonnegative real numbers with $5x+5y/2+5z \le n-1$ is at $x=(n-1)/5$, $y=z=0$. Hence,

$$
w_{-1}(T) \le \frac{n-1}{4}+\frac{11(n-1)}{420}=\frac{29(n-1)}{105}<\frac{5n+8}{18}.
$$

This completes the proof of the theorem. ■

Remark. It is easily seen that $w_{-1}(T)=1$ if and only if $T \cong K_{1,n-1}$. The argument for the upper bound could perhaps be further refined, but the improvement may not be worth the additional effort.

For $n \ge 2$, let $f(n) = \max\{w_{-1}(T)\colon T \text{ is a tree of order } n\}$ and, set $f(0)=f(1)=0$. Then $f(2)=1$ and $f(n)=(n+1)/4$ for $3 \le n \le 8$. Any tree T of order n with $w_{-1}(T)=f(n)$ will be referred to as a **max tree**.

Lemma 2. For all $n \in \mathbb{N}$, $f(n+1) \ge f(n)$.

Proof. Suppose leaf y is adjacent to z in a max tree T of order $n \ge 2$. Let $T' = T + xy$ (where x is a new vertex). Then $f(n+1) \ge w_{-1}(T') = w_{-1}(T) - 1/2d_T(z) + 1/2 \ge w_{-1}(T) = f(n)$. ■

We next show that $f(n)$ is an essentially super-additive function.

Lemma 3. For all $m, n \in \mathbb{N}$, $f(m+n+2) \geq f(m) + f(n)$.

Proof. Our result is readily seen to be true for all $m, n \in \mathbb{N}$ with $m+n \leq 6$. Suppose $m+n \geq 7$. For either $m \leq 1$ or $n \leq 1$, our result follows from Lemma 2, so we assume that $m, n \geq 2$. Let T_1, T_2 be vertex disjoint max trees of order m, n, respectively. Let leaf x_i be adjacent to y_i in T_i; $z_1, \ldots, z_r$ be the other (if any) vertices of T_1 adjacent to y_1; and $w_1, \ldots, w_s$ be the other (if any) vertices of T_2 adjacent to y_2. Let $T = T_1 + T_2 + x_1u + uv + vx_2$ (where u, v are new vertices). Suppose $m = 2$ (and $r = 0$) so $n \geq 5$ (and $s \geq 1$). Now,

$$f(n+4) \geq w_{-1}(T) = w_{-1}(T_2) - \frac{1}{2(s+1)} + \frac{5}{4} \geq w_{-1}(T_2) + 1 = f(m) + f(2),$$

(similarly for $m \geq 5$ and $n = 2$). Suppose $m \geq 3$ (and $r \geq 1$), $n \geq 3$ (and $s \geq 1$). Then,

$$\begin{aligned} f(m+n+2) \geq w_{-1}(T) &= w_{-1}(T_1) + w_{-1}(T_2) - \frac{1}{2(r+1)} - \frac{1}{2(s+1)} + \frac{3}{4} \\ &> w_{-1}(T_1) + w_{-1}(T_2) = f(m) + f(n). \quad \blacksquare \end{aligned}$$

Our next result is a (very) slight extension of Fekete's Lemma [3].

Theorem 4. $\lim_{n \to \infty} f(n)/n$ exists and is a nonnegative real number.

Proof. Fix $m \in \mathbb{Z}^+$. Any integer $n \geq 2$ can be uniquely written as $n = s(m+2) + t + 2$ for appropriate nonnegative integers s, t with $t \leq m+1$. Now Lemmas 2, 3 imply

$$f(n) \geq f(t) + sf(m)$$

so that

$$\frac{f(n)}{n} \geq \frac{f(t)}{n} + \frac{f(m)}{m} - \frac{f(m)(2s+t+2)}{mn}.$$

Hence,

$$\frac{5}{18} \geq \liminf_{n \to \infty} \frac{f(n)}{n} \geq \frac{f(m)}{m} - \frac{2f(m)}{m(m+2)},$$

by Theorem 1 and noting that

$$\lim_{n \to \infty} \frac{2s+t+2}{n} = \frac{2}{m+2}.$$

Then,

$$\frac{5}{18} \geq \liminf_{n\to\infty} \frac{f(n)}{n} \geq \limsup_{m\to\infty} \frac{f(m)}{m},$$

since Theorem 1 implies

$$\lim_{m\to\infty} \frac{2f(m)}{m(m+2)} = 0. \blacksquare$$

The value $K := \lim_{n\to\infty} f(n)/n$ is of interest and appears difficult to evaluate. We next describe the best constructive lower bound we have been able to find.

For an integer $r \geq 2$, T_r denotes the tree obtained from the star $K_{1,r}$ by appending three internally-disjoint paths of length 2 to each leaf of $K_{1,r}$. Then T_r has order $v(T_r) = 7r + 1$ and weight $w_{-1}(T_r) = (15r + 2)/8$, so that $\lim_{r\to\infty} w_{-1}(T_r)/v(T_r) = 15/56$. As a consequence, $0.267857\cdots = 15/56 \leq K \leq 5/18 = 0.277777\cdots$. We also note this implies that paths are not max trees for all sufficiently large n, since $w_{-1}(P_n) = (n+1)/4$ for $n \geq 3$.

III. Expected Value and Variance of the General Randić Index for Simply Generated Families of Trees

Let there be given a sequence $\Gamma = (c_0, c_1, c_2, \ldots)$ of nonnegative constants where $c_0 = 1$. Let $\mathcal{F} = \mathcal{F}_\Gamma$ denote the set of weighted ordered trees such that each ordered tree T is assigned the **weight**

$$c(T) = \prod_{i\geq 0} c_i^{N_i(T)},$$

where $N_i(T)$ denotes the number of vertices of T of out-degree i. We call such a family a **simply generated** family of trees (see, e.g., [5]). Let $\mathcal{F}_n$ denote the subset of trees T in $\mathcal{F}$ such that T has n vertices and let $y_n = \sum_{T\in\mathcal{F}_n} c(T)$. Then the generating function $Y = \sum_1^\infty y_n x^n$ of the family $\mathcal{F}$ satisfies the relation

$$Y = x\Phi(Y) \tag{5}$$

where $\Phi(t) = 1 + \sum_1^\infty c_i x^i$. We note, for later use, that this implies that

$$xY' = (1 - x\Phi'(Y))^{-1}Y. \tag{6}$$

We now determine a relation for the generating function

$$M(x) = \sum_{1}^{\infty} e(n, \alpha) y_n x^n$$

where

$$e(n, \alpha) y_n = \sum_{T \in \mathcal{F}_n} w_\alpha(T) c(T)$$

for any given simply generated family $\mathcal{F}$ of trees and for any fixed value of α. We assign each tree $T \in \mathcal{F}_n$ probability $c(T)/y_n$ so that $e(n, \alpha)$ is the expected value of w_α over $\mathcal{F}_n$.

Theorem 5. Let $F(t) = \sum_{s \geq 0} c_s (s+1)^\alpha t^s$ and $G(t) = \sum_{r \geq 1} c_r r^\alpha t^r$. Then

$$M(x) = x^2 Y^{-1} x Y' F'(Y) F(Y) + x^2 (F'(Y) - G'(Y)) F(Y). \tag{7}$$

Proof. Let $B(x) = \sum_1^\infty b_n x^n$ denote the generating function of the trees in $\mathcal{F}$ with a distinguished leaf, i.e.,

$$b_n = \sum_{T \in \mathcal{F}_n} N_0(T) c(T).$$

It is not difficult to see that $B(x) = x + x\Phi'(Y) B(x)$; this and relation (6) imply that

$$B(x) = x(1 - x\Phi'(Y)) = (x/Y) x Y'. \tag{8}$$

(This is a special case of a more general result proved in [6]; and it is essentially the same result as relation (3.3) in [2].)

Consider any edge uv of a tree T from $\mathcal{F}$ where we may assume that the path from the root of T to v contains u. Let us suppose that u and v have out-degrees r and s, respectively, where $r \geq 1$ and $s \geq 0$. If we remove the r edges incident with u (that lead away from the root) then T falls into (a) an ordered collection of r subtrees one of which is rooted at v and has out-degree s, and (b) a subtree T' rooted at the root of T and in which u is a leaf.

The generating function for trees in which the root has out-degree s is $xc_s Y^s$, so the generating function for collections of trees as described in (a) is $rY^{r-1} xc_s Y^s$. (The factor r is present to account for the fact that the subtree containing v can occur in any one of r possible positions.) The generating function for trees T' with a distinguished leaf u that is **not** the root-vertex is clearly $B(x)-x$. If we join the roots of the trees in an ordered collection of type (a) to the leaf u of such a tree T' then the degrees of u and v in the resulting tree T are $r+1$ and $s+1$, so $w_\alpha(uv) = \big((r+1)(s+1)\big)^\alpha$. When we take this into account, observe that the weight factor associated with the vertex u in T is c_r, and then sum over r and s we find that the contribution to $M(x)$ of all edges uv where u is not the root-vertex is

$$(B(x)-x)\sum_{r\geq 1} rc_r(r+1)^\alpha Y^{r-1}\cdot x\sum_{s\geq 0} c_s(s+1)^\alpha Y^s$$
$$= x(B(x)-x)F'(Y)F(Y). \tag{9}$$

Now suppose that the vertex u is the root-vertex of T', i.e., that T' is the trivial tree consisting of the single vertex u. This time when we join the roots of the trees in an ordered collection of type (a) to u the degrees of u and v in the resulting tree T are r and $s+1$, so $w_\alpha(uv) = \big(r(s+1)\big)^\alpha$. Continuing as before, we find that the contribution to $M(x)$ of all edges uv where u is the root-vertex is

$$x\sum_{r\geq 1} rc_r r^\alpha Y^{r-1}\cdot x\sum_{s\geq 0} c_s(s+1)^\alpha Y^s = x^2G'(Y)F(Y). \tag{10}$$

The required relation (7) now follows from relations (8), (9), and (10). ■

Before stating the general asymptotic behaviour of $e(n,\alpha)$ we impose some technical conditions, namely, that the function $\Phi(t)$ that appears in relation (5) is analytic in the disk $|t| < R \leq \infty$ and that

$c_i \geq 0$ for $i \geq 1$ and $c_i > 0$ for some $i > 1$;

$gcd\{i\colon i \geq 1 \text{ and } c_i > 0\} = 1$; and

$\tau\Phi'(\tau) = \Phi(\tau)$ for some τ, where $0 < \tau < R$.

It follows from these assumptions (see [5] or [8]) that τ is unique and that $Y(x)$ is analytic in the disk $|x| \leq \rho = \tau/\Phi(\tau)$ except at $x=\rho$; furthermore, $Y(x)$ has an expansion in the neighborhood of ρ of the form

$$Y(x) = \tau - b(\rho - x)^{1/2} - b_2(\rho - x) - \cdots \tag{11}$$

where $b = \Phi(\tau)\big(2/\tau\Phi''(\tau)\big)^{1/2}$. Hence, by Darboux's theorem (cf. [10; p. 150]),

$$y_n = a\rho^{-n}n^{-3/2}(1+O(n^{-1})) \tag{12}$$

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

Corollary 6. For any fixed α,

$$e(n,\alpha) = \rho^2\tau^{-1}F'(\tau)F(\tau)n + O(1) \text{ as } n \to \infty. \tag{13}$$

Proof. The functions $F(t)$ and $G(t)$ are analytic in the disk $|t| < R$ where $\tau = Y(\rho) < R$, in view of our assumptions about the function $\Phi(t)$. The required conclusion follows readily from relation (7) and expansion (11) upon appealing to Darboux's theorem. ■

By an extension of the foregoing arguments, we can find the variance $\sigma^2(n,\alpha)$ of w_α over $\mathcal{F}_n$.

Theorem 7. For any fixed α, there exists a positive constant c_α with

$$\sigma^2(n,\alpha) = c_\alpha n^{3/2} + O(n) \text{ as } n \to \infty.$$

It follows from Chebyshev's inequality that the distribution of w_α becomes increasingly concentrated around its mean as n increases.

We now find $e(n,\alpha)$ or $L_\alpha := \lim_{n\to\infty} e(n,\alpha)/n$ when $\alpha = -1$ or 1 for certain families of trees.

$\alpha = -1$. In this case, $F(t) = \sum c_s(s+1)^{-1}t^s$ and

$$F'(t) = \sum \{1 - (s+1)^{-1}\}c_s t^{s-1} = \frac{\Phi(t)}{t} - \frac{F(t)}{t}.$$

Therefore,

$$\begin{aligned} L_{-1} = \rho^2\tau^{-1}F(\tau)F'(\tau) &= \frac{\rho F(\tau)}{\tau}\left\{\frac{\rho\Phi(\tau)}{\tau} - \frac{\rho F(\tau)}{\tau}\right\} \\ &= \frac{F(\tau)}{\Phi(\tau)}\left\{1 - \frac{F(\tau)}{\Phi(\tau)}\right\}. \end{aligned} \tag{14}$$

Consequently, $L_{-1} \le 1/4$ for all families satisfying our assumptions. In fact it is not difficult to show that for such families $2F(\tau) > \Phi(\tau)$ so that $L_{-1} < 1/4$.

Consider the family $\mathcal{F}$ for which $\Phi(t) = 1 + \gamma t + (\beta t)^k/(k-1)$ for some positive constants γ and β and some integer $k \ge 2$. Then $\tau = 1/\beta$ and

$$\frac{F(\tau)}{\Phi(\tau)} = \frac{\gamma(k^2-1) + 2\beta k^2}{2\gamma(k^2-1) + 2\beta k(k+1)}. \tag{15}$$

This tends to $k/(k+1)$ as $\gamma \to 0$ which is arbitrarily close to 1 for large values of k; and this quantity tends to 1/2 as $\beta \to 0$. So $F(\tau)/\Phi(\tau)$ can take on any value between 1/2 and 1 and, consequently, L_{-1} can take on **any** value between 0 and 1/4. (We could regard the collection of paths as a limiting extreme case with $c_2 = c_3 = \cdots = 0$.)

If $\mathcal{F}$ is the family of rooted labelled trees then $\Phi(t) = e^t$, $\tau = 1$ and $F(t) = (e^t - 1)/t$. Hence, $F(\tau)/\Phi(\tau) = (e-1)/e$ and

$$L_{-1} = e^{-1} - e^{-2} = 0.232544\cdots. \tag{16}$$

In fact, for this family it can be shown that

$$e(n,-1) = n\left\{\left(1-\frac{1}{n}\right)^{n-1} - \left(1-\frac{2}{n}\right)^{n-1}\right\}. \tag{17}$$

If $\mathcal{F}$ is the family of ordinary ordered trees then $\Phi(t) = (1-t)^{-1}$, $\tau = 1/2$ and $F(t) = t^{-1}\log\big(1/(1-t)\big)$. Hence, $F(\tau)/\Phi(\tau) = \log 2$ and

$$L_{-1} = \log 2(1-\log 2) = 0.212694\cdots. \tag{18}$$

$\boldsymbol{\alpha = 1.}$ In this case,

$$F(t) = \sum (s+1)c_s t^s = t\Phi'(t) + \Phi(t)$$

and

$$F'(t) = 2\Phi'(t) + t\Phi''(t).$$

When we substitute these expressions in (13) and recall that $\rho\Phi(\tau) = \tau$ and $\rho\Phi'(\tau) = 1$, we find that

$$\begin{aligned} L_1 &= \tau^{-1}\rho F(\tau)\rho F'(\tau) \\ &= \tau^{-1}\big(\tau\rho\Phi'(\tau) + \rho\Phi(\tau)\big)\big(2\rho\Phi'(\tau) + \rho\tau\Phi''(\tau)\big) \\ &= 2(2+A), \end{aligned} \tag{19}$$

where $A = \rho\tau\Phi''(\tau)$. The quantity A can take on any positive value (see [5; p. 1005]), so L_1 can take on **any** value greater than 4. (Again, paths can be regarded as a limiting extreme case.)

If $\mathcal{F}$ is the family of rooted labelled trees, then it can be shown that

$$e(n,1) = (n-1)\left(6 - \frac{16}{n} + \frac{12}{n^2}\right), \tag{20}$$

and, if $\mathcal{F}$ is the family of ordinary plane trees, then

$$e(n,1) = 4(n-1)\frac{(2n-1)(n-1)}{(n+1)(n+2)}. \tag{21}$$

If $\mathcal{F}$ is the family of binary trees, then an explicit formula for the expected value of $w_\alpha(T)$ for all α follows readily from first principles. We observe that of the

$$y_{2n+1} = \frac{1}{n+1}\binom{2n}{n}$$

rooted binary trees with n vertices of out-degree 2 and $n+1$ leaves, there are $2y_{2n-1}$ trees in which the root is joined to a leaf and $y_{2n+1} - 2y_{2n-1}$ in which it is not, for $n \geq 2$. Any edge of a non-trivial binary tree must have weight 1/2, 1/3, 1/6, or 1/9 and it is not difficult to count the number of edges with these weights in the two types of trees just described. In this way we find that

$$e(2n+1,\alpha) = \left\{(n-2)9^\alpha + (n+1)3^\alpha + 2\cdot 6^\alpha\right\} + \frac{n+1}{2n-1}\left\{9^\alpha - 6^\alpha - 3^\alpha + 2^\alpha\right\} \tag{22}$$

for $n \geq 1$. In particular,

$$e(2n+1,-1) = \frac{8n^2+3n-2}{9(2n-1)}$$

and

$$e(2n+1,1) = \frac{24n^2-34n+14}{2n-1}.$$

IV. Conclusion

We conclude with several questions that may be of interest.

(1) Find $K = \lim_{n\to\infty} f(n)/n$. We know that $15/56 \leq K \leq 5/18$ and suspect that the lower bound is closer to K than the upper bound.

(2) Refine the upper bound in Theorem 1 for $w_{-1}(T)$ so that it is sharp for infinitely-many values of n.

(3) Find the asymptotic distribution of w_{-1} over the class of labelled trees of order n as $n \to \infty$.

References

1. B. Bollobás and P. Erdös, Graphs of extremal weights, *Ars Combinatoria* **50** (1998), 225–233.
2. L.H. Clark, A. Meir and J.W. Moon, On the Steiner distance of trees from certain families, to appear in *Australasian Journal of Combinatorics.*
3. M. Fekete, Über die verteilung der wurzeln bei gewissen algebraischen gleichungen mit ganzzahligen koeffizienten, *Mathematische Zeitschrift* **17** (1923), 228–249.
4. L.B. Kier and L.H. Hall, *Molecular Connectivity in Chemistry and Drug Research,* Academic Press, San Francisco, 1976.
5. A. Meir and J.W. Moon, On the altitude of nodes in random trees, *Canadian Journal of Mathematics* **30** (1978), 997–1015.
6. A. Meir and J.W. Moon, On nodes of out-degree one in random trees, *Colloq. Math. Soc. János Bolyai* **52** (1987), 405–416.
7. M. Randić, On characterization of molecular branching, *Journal of the American Chemical Society* **97** (1975), 6609–6615.
8. J.–M. Steyaert and P. Flajolet, Patterns and pattern-matching in trees: an analysis, *Information and Control* **58** (1983), 19–58.
9. D.B. West, *Introduction to Graph Theory,* Prentice-Hall, Upper Saddle River, NJ, 1996.
10. H.S. Wilf, *Generatingfunctionology,* Academic Press, San Diego, 1990.
11. P. Yu, An upper bound on the randic of trees, *Journal of Mathematical Study* (Chinese) **31** (1998), 225–230.