On the average Wiener index of degree-restricted trees. *

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Abstract

The Wiener index, defined as the total sum of distances in a graph, is one of the most popular graph-theoretical indices. Its average value has been determined for several classes of trees, giving an asymptotics of the form $Kn^{5/2}$ for some K. In this note, it is shown how the method can be extended to trees with restricted degrees. Particular emphasis is placed on chemical trees – trees with maximal degree ≤ 4 – since the Wiener index is of interest in theoretical chemistry.

1 Introduction

The Wiener index of a graph G, named after the chemist Harold Wiener [17], who considered it in connection with paraffin boiling points, is given by

$$\sum_{\{v,w\}\subseteq V(G)} d_G(v,w), \tag{1}$$

where d_G denotes the distance in G. Besides its purely graph-theoretic value, the Wiener index has interesting applications in chemistry. We quote [2], which gives an extensive summary on the various works, and refer to [16] for further information on the chemical applications.

The average behaviour of the Wiener index was first studied by Entringer et al. [5], who considered so-called simply generated families of trees (introduced by Meir and Moon, cf. [9]). They were able to prove that the average Wiener index is asymptotically $Kn^{5/2}$, where the constant K depends on the specific family of trees. Thus, the average value of

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the Wiener index is, apart from a constant factor, the geometric mean of the extremal values, which are given for the star S_n and the path P_n respectively:

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

for all trees T with n vertices (s. [4]). In more recent articles, Neininger [11] studied recursive and binary search trees, and Janson [7] determined moments of the Wiener index of random rooted trees.
Dobrynin and Gutman [3] calculated numerical values for the average Wiener index of trees and chemical trees of small order by direct computer calculation.
The average Wiener index of a tree (taking isomorphies into account) has been determined, in a different context, in a paper of Moon [10] – it is given asymptotically by $0.56828n^{5/2}$.
The aim of this note is to extend the cited result to trees with restricted degree, especially chemical trees. In fact, the enumeration method for chemical trees is older than the result of Otter and goes back to Cayley (cf. [1]) and Pólya [13].
Let $Z(A)$ denote the cycle index of a permutation group A, and write $Z(A, f(z))$ for the cycle index $Z(A)$ with $f(z^l)$ substituted for the variable s_l belonging to an l-cycle. If $T_{\mathcal{G}}(z)$ and $T_{\mathcal{G}_k}(z)$ are the counting series for two classes $\mathcal{G}$, $\mathcal{G}_k$ of rooted trees, where $\mathcal{G}_k$ is constructed by attaching a collection of k trees from the family $\mathcal{G}$ to a common root (ignoring the order), we have (cf. [6])

$$T_{\mathcal{G}_k}(z) = z \cdot Z(S_k, T_{\mathcal{G}}(z)), \tag{3}$$

where S_k denotes the symmetric group. Additionally, we define $Z(S_0, f(z)) = 1$ and $Z(S_k, f(z)) = 0$ for $k < 0$. This gives us, for example, the functional equation for the counting series $T_3(z)$ of rooted trees with maximal outdegree ≤ 3:

$$T_3(z) = z \cdot \sum_{k=0}^{3} Z(S_k, T_3(z)).$$

2 Functional equations for the total height and Wiener index

Our method will be the same one as in Entringer et al. [5]. First, we consider an auxiliary value, $D(T)$, denoting the sum of the distances of all vertices from the root. This is also known as the *total height* of the tree T, cf. [14].
The value $D(T)$ can be calculated recursively from the branches $T_1, \ldots, T_k$ of T, viz.

$$D(T) = \sum_{i=1}^{k} D(T_i) + |T| - 1, \tag{4}$$

where $|T|$ is the size (number of vertices) of T. Now we have to translate this recursive property into a functional equation. Again, we suppose that the branches come from a certain family $\mathcal{G}$, and denote the corresponding generating function for $D(T)$ by

$$D_{\mathcal{G}}(z) = \sum_{T \in \mathcal{G}} D(T) z^{|T|}.$$

Let $\mathcal{G}_k$ be defined as before and define $D_{\mathcal{G}_k}(z)$ analogously. There is an obvious bijection between the elements of $\mathcal{G}_{k-j}$ and the elements of $\mathcal{G}_k$ which contain a certain tree $T \in \mathcal{G}$ at least j times as a branch. Therefore, if $g_{k,n}$ denotes the number of trees of size n in $\mathcal{G}_k$, the branch B appears

$$\sum_{j=1}^{k} g_{k-j,n-j|B|}$$

times in all rooted trees of size n belonging to $\mathcal{G}_k$. Together with (4), this gives us

$$\begin{aligned} D_{\mathcal{G}_k}(z) &= \sum_{B\in\mathcal{G}} D(B) \sum_{j=1}^{k} \sum_{n\geq 1} g_{k-j,n-j|B|} z^n + zT'_{\mathcal{G}_k}(z) - T_{\mathcal{G}_k}(z) \\ &= z\sum_{j=1}^{k} D_{\mathcal{G}}(z^j) Z(S_{k-j}, T_{\mathcal{G}}(z)) + zT'_{\mathcal{G}_k}(z) - T_{\mathcal{G}_k}(z). \end{aligned} \tag{5}$$

Similarly, we introduce generating functions for the Wiener index:

$$W_{\mathcal{G}}(z) = \sum_{T\in\mathcal{G}} W(T) z^{|T|},$$

and $W_{\mathcal{G}_k}(z)$ is defined analogously. Now, we use the following recursive relation from [5], which relates the Wiener index of a rooted tree T with the Wiener indices of its branches $T_1, \dots, T_k$:

$$W(T) = D(T) + \sum_{i=1}^{k} W(T_i) + \sum_{i\neq j} \Big(D(T_i) + |T_i|\Big)|T_j|, \tag{6}$$

where the last sum goes over all $k(k-1)$ pairs of different branches. Now, we have to determine the number of times the pair $(B_1, B_2) \in \mathcal{G}^2$ appears in trees with n vertices belonging to $\mathcal{G}_k$. By the same argument that was applied before, this number is given by

$$\sum_{j=1}^{k-1} \sum_{i=1}^{k-j} g_{k-j-i,n-j|B_1|-i|B_2|}$$

if B_1 and B_2 are distinct elements from $\mathcal{G}$. If, on the other hand, $B_1 = B_2 = B$ are equal, the number is

$$\sum_{j=1}^{k} j(j-1)\Big(g_{k-j,n-j|B|} - g_{k-j-1,n-(j+1)|B|}\Big) = \sum_{j=1}^{k} 2(j-1) g_{k-j,n-j|B|}.$$

Together with (6), this yields

$$\begin{aligned} W_{\mathcal{G}_k}(z) = D_{\mathcal{G}_k}(z) &+ \sum_{B\in\mathcal{G}} W(B) \sum_{j=1}^{k} \sum_{n\geq 1} g_{k-j,n-j|B|} z^n \\ &+ \sum_{B_1\in\mathcal{G}} \sum_{B_2\in\mathcal{G}} \Big(D(B_1) + |B_1|\Big)|B_2| \sum_{j=1}^{k-1} \sum_{i=1}^{k-j} \sum_{n\geq 1} g_{k-j-i,n-j|B_1|-i|B_2|} z^n \\ &+ \sum_{B\in\mathcal{G}} \Big(D(B) + |B|\Big)|B| \sum_{j=1}^{k} \sum_{n\geq 1} (j-1) g_{k-j,n-j|B|} z^n \end{aligned}$$

or

$$
\begin{aligned}
W_{\mathcal{G}_k}(z) = D_{\mathcal{G}_k}(z) &+ z\sum_{j=1}^{k} W_{\mathcal{G}}(z^j) Z(S_{k-j}, T_{\mathcal{G}}(z)) \\
&+ z\sum_{j=1}^{k-1}\sum_{i=1}^{k-j}\Big(D_{\mathcal{G}}(z^j) + z^j T'_{\mathcal{G}}(z^j)\Big)\cdot z^i T'_{\mathcal{G}}(z^i) Z(S_{k-j-i}, T_{\mathcal{G}}(z)) \qquad (7)\\
&+ z\sum_{j=1}^{k}(j-1)z^j\Big(D'_{\mathcal{G}}(z^j) + T'_{\mathcal{G}}(z^j) + z^j T''_{\mathcal{G}}(z^j)\Big) Z(S_{k-j}, T_{\mathcal{G}}(z)).
\end{aligned}
$$

These functional equations (and combinations of them for different values of k) enable us to calculate the average Wiener indices for various sorts of degree-restricted rooted trees. For the study of unrooted trees, however, we need yet another tool. In particular, we want to determine the average Wiener index of trees with maximal degree ≤ 4, also known as chemical trees (cf. [3]).

For this purpose, let $\mathcal{F}_{\mathcal{D}}$ denote the family of rooted trees with the property that the outdegree of every vertex lies in $\mathcal{D}_0 = \mathcal{D} \cup \{0\}$, where $\mathcal{D} \subseteq \mathbb{N}$, and let $\tilde{\mathcal{F}}_{\mathcal{D}}$ be the family of trees with the property that all degrees lie in the set $\tilde{\mathcal{D}} = \{d+1 : d \in \mathcal{D}_0\}$. By a theorem of Otter (cf. [6]), the number of different representations of a tree as a rooted tree equals 1 plus the number of representations as a pair of two unequal rooted trees (the order being irrelevant), with their roots joined by an edge. Thus, for counting the trees in $\tilde{\mathcal{F}}_{\mathcal{D}}$, one has to take

- rooted trees with $k \in \tilde{\mathcal{D}}$ branches from $\mathcal{F}_{\mathcal{D}}$

minus

- pairs of unequal rooted trees from $\mathcal{F}_{\mathcal{D}}$, joined by an edge.

If $T_{\mathcal{D}}$ and $\tilde{T}_{\mathcal{D}}$ are the respective generating functions for the number of trees in $\mathcal{F}_{\mathcal{D}}$ and $\tilde{F}_{\mathcal{D}}$, this means that

$$
\tilde{T}_{\mathcal{D}}(z) = z + z\sum_{k\in\mathcal{D}_0} Z(S_{k+1}, T_{\mathcal{D}}(z)) - \frac{1}{2}\Big(T_{\mathcal{D}}^2(z) - T_{\mathcal{D}}(z^2)\Big). \qquad (8)
$$

The first summand, corresponding to the tree with only a single vertex, can be included or not, as it makes no real difference. The generating function for the Wiener index of trees from $\tilde{\mathcal{F}}_{\mathcal{D}}$ is also a difference of the respective generating functions for the two possibilities of representing a tree from $\tilde{\mathcal{F}}_{\mathcal{D}}$ which were given above. If we denote it by $\tilde{W}_{\mathcal{D}}(z) = \tilde{W}_{\mathcal{D}}^{(1)}(z) - \tilde{W}_{\mathcal{D}}^{(2)}(z)$, the first summand is given by equation (9), which is easily deduced from (5) and (7).

$$\begin{aligned}\tilde{W}^{(1)}_{\mathcal{D}}(z) = \sum_{k\in\tilde{D}} \Bigg(& z\sum_{j=1}^{k} D_{\mathcal{D}}(z^j) Z(S_{k-j}, T_{\mathcal{D}}(z)) + z\left(\frac{d}{dz} z\cdot Z(S_k, T_{\mathcal{D}}(z))\right) - z\cdot Z(S_k, T_{\mathcal{D}}(z)) \\ & + z\sum_{j=1}^{k} W_{\mathcal{D}}(z^j) Z(S_{k-j}, T_{\mathcal{D}}(z)) \\ & + z\sum_{j=1}^{k-1}\sum_{i=1}^{k-j}\Big(D_{\mathcal{D}}(z^j) + z^j T'_{\mathcal{D}}(z^j)\Big)\cdot z^i T'_{\mathcal{D}}(z^i) Z(S_{k-j-i}, T_{\mathcal{D}}(z)) \\ & + z\sum_{j=1}^{k}(j-1)z^j\Big(D'_{\mathcal{D}}(z^j) + T'_{\mathcal{D}}(z^j) + z^j T''_{\mathcal{D}}(z^j)\Big) Z(S_{k-j}, T_{\mathcal{D}}(z))\Bigg),\end{aligned} \tag{9}$$

On the other hand, if two rooted trees T_1 and T_2 are joined by an edge, the Wiener index of the resulting tree T is given by

$$W(T) = W(T_1) + W(T_2) + D(T_1)|T_2| + D(T_2)|T_1| + |T_1||T_2|.$$

Therefore, we obtain

$$\begin{aligned}\tilde{W}^{(2)}_{\mathcal{D}}(z) &= \frac{1}{2}\sum_{T_1\in\mathcal{F}_{\mathcal{D}}}\sum_{T_2\in\mathcal{F}_{\mathcal{D}}}\Big(W(T_1) + W(T_2) + D(T_1)|T_2| + D(T_2)|T_1| + |T_1||T_2|\Big) z^{|T_1|+|T_2|} \\ &\quad - \frac{1}{2}\sum_{T\in\mathcal{F}_{\mathcal{D}}}\Big(2W(T) + 2D(T)|T| + |T|^2\Big) z^{2|T|} \\ &= \frac{1}{2}\Big(2W_{\mathcal{D}}(z)T_{\mathcal{D}}(z) + 2D_{\mathcal{D}}(z)\cdot zT'_{\mathcal{D}}(z) + z^2 T'_{\mathcal{D}}(z)^2 \\ &\quad - 2W_{\mathcal{D}}(z^2) - 2z^2 D'_{\mathcal{D}}(z^2) - z^2(z^2 T''_{\mathcal{D}}(z^2) + T'_{\mathcal{D}}(z^2))\Big).\end{aligned} \tag{10}$$

3 Wiener index of trees and chemical trees

Equations (5), (7), (9) and (10) enable us to calculate the exact average Wiener index of all trees of size n from a certain family $\mathcal{F}$ with degree restrictions for considerably high n. As an example, we calculate the average Wiener index of all chemical trees (i.e. maximal degree ≤ 4) up to $n = 100$. We have to start with the generating function T_3 for $\mathcal{F}_3$, the class of rooted trees with maximal outdegree ≤ 3, whose functional equation is given by

$$T_3(z) = z\cdot\sum_{k=0}^{3} Z(S_k, T_3(z)).$$

Then, the generating function for the number of trees with degree ≤ 4 is given by

$$\tilde{T}_3(z) = z\sum_{k=0}^{4} Z(S_k, T_3(z)) - \frac{1}{2}\Big(T_3^2(z) - T_3(z^2)\Big).$$

From (5), we know that the corresponding generating function for $D(T)$ satisfies

$$D_3(z) = z\sum_{k=1}^{3}\sum_{j=1}^{k} D_3(z^j)Z(S_{k-j}, T_3(z)) + zT_3'(z) - T_3(z).$$

Analogously, from (7), we obtain

$$\begin{aligned} W_3(z) = D_3(z) + \sum_{k=1}^{3}\Bigg(& z\sum_{j=1}^{k} W_3(z^j)Z(S_{k-j}, T_3(z)) \\ & + z\sum_{j=1}^{k-1}\sum_{i=1}^{k-j}\Big(D_3(z^j) + z^jT_3'(z^j)\Big)\cdot z^iT_3'(z^i)Z(S_{k-j-i}, T_3(z)) \\ & + z\sum_{j=1}^{k}(j-1)z^j\Big(D_3'(z^j) + T_3'(z^j) + z^jT_3''(z^j)\Big)Z(S_{k-j}, T_3(z))\Bigg). \end{aligned}$$

$\tilde{W}_3$, the generating function for the sum of the Wiener indices of all trees with maximal degree ≤ 4, is then given by (9) and (10). Easy computer calculations yield us the following table – up to $n = 20$, the values were given in [3] by direct computation; $\tilde{t}_{4,n}$ denotes the number of trees of size n with maximal degree ≤ 4, $\tilde{w}_{4,n}$ the total of their Wiener indices:

n	$\tilde{t}_{4,n}$	$\tilde{w}_{4,n}$	$\tilde{w}_{4,n}/\tilde{t}_{4,n}$
1	1	0	0
2	1	1	1
3	1	4	4
4	2	19	9.5
5	3	54	18
6	5	155	31
7	9	432	48
8	18	1252	69.56
9	35	3384	96.69
10	75	9714	129.52
20	366319	310884129	848.67
50	$1.11774 \cdot 10^{18}$	$1.05659 \cdot 10^{22}$	9452.93
100	$5.92107 \cdot 10^{39}$	$3.34957 \cdot 10^{44}$	56570.38

Table 1: Some numerical values for chemical trees.

Things are somewhat easier in the case of ordinary trees. If $\mathcal{D} = \mathbb{N}$, the functional equations reduce to

$$D(z) = T(z)\sum_{j\geq 1} D(z^j) + zT'(z) - T(z),$$

$$
\begin{aligned}
W(z) &= D(z) + T(z)\sum_{j\ge 1} W(z^j) + \sum_{j\ge 1}\sum_{i\ge 1}\Big(D(z^j) + z^j T'(z^j)\Big)\cdot z^i T'(z^i)\cdot T(z) \\
&\quad + \sum_{j\ge 1}(j-1)z^j\Big(D'(z^j) + T'(z^j) + z^j T''(z^j)\Big)\cdot T(z), \\
\tilde{W}(z) &= W(z) - \frac{1}{2}\Big(2W(z)T(z) + 2D(z)\cdot zT'(z) + z^2T'(z)^2 \\
&\quad - 2W(z^2) - 2z^2D'(z^2) - z^2(z^2T''(z^2) + T'(z^2))\Big).
\end{aligned}
$$

These equations are also given in Moon [10]. They yield the following table of values:

n	w_n	$\tilde{w}_n$	w_n/t_n	$\tilde{w}_n/\tilde{t}_n$
1	0	0	0	0
2	1	1	1	1
3	8	4	4	4
4	38	19	9.5	9.5
5	164	54	18.22222	18
6	609	180	30.45	30
7	2256	508	47	46.18182
8	7815	1533	67.95652	66.65217
9	26892	4332	94.02797	92.17021
10	90146	13041	125.37691	123.02830
20	10319401978	655274837	804.55470	796.13984
50	$3.73537\cdot 10^{24}$	$9.20871\cdot 10^{22}$	8768.95009	8732.57790
100	$2.66359\cdot 10^{48}$	$3.25933\cdot 10^{46}$	51836.59972	51724.32112

Table 2: Some numerical values for trees.

4 Asymptotic analysis

Now, we study the asymptotic behavior of the Wiener index for rooted trees and trees with degree restrictions. In particular, we will prove the following fairly general theorem:

Theorem 1 *Let $\mathcal{D}\subseteq\mathbb{N}$ be an arbitrary subset of the positive integers such that $\mathcal{D}\ne\{1\}$ and $\gcd(d : d\in\mathcal{D}) = 1$. Then the average total height $D(T_n)$ of a tree $T_n\in\mathcal{F}_{\mathcal{D}}$ with n vertices is asymptotically $2Kn^{3/2}$, the average Wiener index is asymptotically $Kn^{5/2}$, where K is given by*

$$
K = \frac{\sqrt{\pi}}{2\alpha b\rho^{3/2}}
$$

and α, b and ρ are defined as follows:

- *ρ is the radius of convergence of $T_{\mathcal{D}}(z)$,*
- *The expansion of $T_{\mathcal{D}}(z)$ around ρ is given by*

$$
T_{\mathcal{D}}(z) = t_0 - b\sqrt{\rho - z} + O(\rho - z), \tag{11}
$$

- $\alpha = \sum_{k\in\mathcal{D}} Z(S_{k-2}, T_{\mathcal{D}}(z))|_{z=\rho}$.

REMARK: If $\mathcal{D} = \mathbb{N}$, we have $\alpha = \frac{1}{\rho} = 2.95576528\ldots$, $\rho = 0.33832185\ldots$ and $b = 2.68112814\ldots$, the constants given by Otter [12].

In the proof of the theorem, we will make use of the following property of the cycle indices of symmetric groups:

Lemma 2 If the cycle index $Z(S_k)$ of the symmetric group S_k is written in terms of $s_1, s_2, \ldots$, we have

$$\frac{\partial}{\partial s_l} Z(S_k) = \frac{1}{l} Z(S_{k-l}).$$

Proof: From [6], we know that the cycle index of S_k has the explicit representation

$$Z(S_k) = \frac{1}{k!} \sum_{(j)} h(j) \prod_{r=1}^{k} s_r^{j_r},$$

where the sum runs over all partitions $(j) = (j_1, \ldots, j_k)$ of k (j_r denotes the number of parts equal to r) and $h(j)$ is given by

$$h(j) = \frac{k!}{\prod_{r=1}^{k} r^{j_r} j_r!}.$$

There is an obvious bijection between the partitions of k which contain l and the partitions of $k-l$. For a partition (j) of k that contains l, let (j') be the partition of $k-l$ which results from replacing j_l by $j_l - 1$. Then it is easy to see that

$$h(j') = \frac{(k-l)! l j_l h(j)}{k!}.$$

This shows that

$$\begin{aligned}
\frac{\partial}{\partial s_l} Z(S_k) &= \frac{1}{k!} \sum_{(j)} \frac{j_l h(j)}{s_l} \prod_{r=1}^{k} s_r^{j_r} \\
&= \frac{1}{(k-l)!} \sum_{(j')} \frac{h(j')}{l} \prod_{r=1}^{k} s_r^{j'_r} = \frac{1}{l} Z(S_{k-l}).
\end{aligned}$$

□

Corollary 3

$$\frac{d}{dz} Z(S_k, f(z)) = \sum_{l=1}^{k} z^{l-1} f'(z^l) Z(S_{k-l}, f(z)).$$

Proof: This follows trivially upon application of the chain rule. □

Proof of the theorem: We fix $\mathcal{D}$ and use the abbreviations T, D, W for $T_{\mathcal{D}}$, $D_{\mathcal{D}}$, $W_{\mathcal{D}}$. We start with the equation

$$T(z) = z \sum_{k\in\mathcal{D}_0} Z(S_k, T(z)). \tag{12}$$

The gcd-condition for $\mathcal{D}$ ensures that all but finitely many coefficients of T are positive. Following [6, pp. 208–214], one can prove that T has positive radius of convergence $1 > \rho \geq 0.33832\ldots$ (the lower bound being given by the case $\mathcal{D} = \mathbb{N}$), that T converges at $z = \rho$ and that ρ is the only singularity on the circle of convergence. Furthermore, T has an expansion of the form (11) around ρ, giving an asymptotic formula for the number $t_{\mathcal{D},n}$ of trees of size n in $\mathcal{F}_{\mathcal{D}}$:

$$t_{\mathcal{D},n} \sim \frac{b}{2\sqrt{\pi}} \rho^{-n+1/2} n^{-3/2}.$$

The values of ρ, t_0 and b can be determined numerically. Differentiating (12) yields, by Corollary 3,

$$\begin{aligned} T'(z) &= \frac{T}{z} + z \sum_{k\in\mathcal{D}} \sum_{l=1}^{k} z^{l-1} T'(z^l) Z(S_{k-l}, T(z)) \\ &= \frac{T}{z} + zT'(z) \sum_{k\in\mathcal{D}} Z(S_{k-1}, T(z)) + \sum_{k\in\mathcal{D}} \sum_{l=2}^{k} z^l T'(z^l) Z(S_{k-l}, T(z)) \end{aligned}$$

and thus

$$T'(z) \left(1 - z \sum_{k\in\mathcal{D}} Z(S_{k-1}, T(z)) \right) = \frac{T}{z} + \sum_{k\in\mathcal{D}} \sum_{l=2}^{k} z^l T'(z^l) Z(S_{k-l}, T(z)). \tag{13}$$

We set

$$\beta := \sum_{k\in\mathcal{D}} \sum_{l=2}^{k} z^l T'(z^l) Z(S_{k-l}, T(z)) \Big|_{z=\rho}.$$

Note, at this occasion, that $T(z^l)$ is holomorphic within a larger circle than $T(z)$ if $l > 1$, and that the sum over l can be uniformly bounded by a geometric sum on any compact subset of this larger circle. Furthermore, since it is a well-known fact that

$$\sum_{k\geq 0} Z(S_k, f(z)) = \exp\left(\sum_{m\geq 1} \frac{1}{m} f(z^m) \right),$$

we know that the sum over all $k \in \mathcal{D}$ converges as the sum $\sum_{m\geq 1} \frac{1}{m} T(\rho^m)$ is bounded. This argument will be used quite frequently in the following steps without being mentioned explicitly. Now, expanding around ρ gives us

$$1 - z \sum_{k\in\mathcal{D}} Z(S_{k-1}, T(z)) \sim \frac{2}{b} \left(\frac{t_0}{\rho} + \beta \right) \sqrt{\rho - z}. \tag{14}$$

On the other hand, we have

$$\begin{aligned} \frac{d}{dz} \left(1 - z \sum_{k\in\mathcal{D}} Z(S_{k-1}, T(z)) \right) &= - \sum_{k\in\mathcal{D}} Z(S_{k-1}, T(z)) - zT'(z) \sum_{k\in\mathcal{D}} Z(S_{k-2}, T(z)) \\ &\quad - z \sum_{k\in\mathcal{D}} \sum_{l=2}^{k-1} z^{l-1} T'(z^l) T(S_{k-1-l}, T(z)). \end{aligned}$$

The first and the last summand are bounded, therefore, if we set

$$\alpha := \sum_{k\in\mathcal{D}} Z(S_{k-2}, T(z))\Big|_{z=\rho},$$

we obtain

$$\frac{d}{dz}\left(1 - z\sum_{k\in\mathcal{D}} Z(S_{k-1}, T(z))\right) \sim -\frac{\rho b\alpha}{2}(\rho - z)^{-1/2},$$

giving us $\alpha = \frac{2}{b^2\rho}\left(\frac{t_0}{\rho} + \beta\right)$. Next, we turn to the functional equation for $D(z)$:

$$D(z) = zT'(z) - T(z) + zD(z)\sum_{k\in\mathcal{D}} Z(S_{k-1}, T(z)) + z\sum_{k\in\mathcal{D}}\sum_{l=2}^{k} D(z^l)Z(S_{k-l}, T(z)). \quad (15)$$

The last summand is bounded around ρ – note that $D(z)$ has the same radius of convergence as $T(z)$, since $D(T) \leq \frac{|T|(|T|-1)}{2}$ for all trees T; the same argument holds true for the generating function of the Wiener index by inequality (2). Solving for $D(z)$ yields

$$D(z) = \frac{zT'(z) - T(z) + z\sum_{k\in\mathcal{D}}\sum_{l=2}^{k} D(z^l)Z(S_{k-l}, T(z))}{1 - z\sum_{k\in\mathcal{D}} Z(S_{k-1}, T(z))}.$$

Therefore, the expansion of $D(z)$ around ρ is given by

$$D(z) \sim \frac{b^2\rho^2}{4(t_0 + \beta\rho)}(\rho - z)^{-1} = \frac{1}{2\alpha}(\rho - z)^{-1}, \quad (16)$$

which follows upon combining (11), (14) and (15). Finally, we consider the function $W(z)$:

$$\begin{aligned} W(z) = D(z) &+ zW(z)\sum_{k\in\mathcal{D}} Z(S_{k-1}, T(z)) + z\sum_{k\in\mathcal{D}}\sum_{j=2}^{k} W(z^j)Z(S_{k-j}, T(z)) \\ &+ z\sum_{k\in\mathcal{D}}\sum_{j=1}^{k-1}\sum_{i=1}^{k-j}\left(D(z^j) + z^jT'(z^j)\right)\cdot z^iT'(z^i)Z(S_{k-j-i}, T(z)) \quad (17) \\ &+ z\sum_{k\in\mathcal{D}}\sum_{j=1}^{k}(j-1)z^j\left(D'(z^j) + T'(z^j) + z^jT''(z^j)\right)Z(S_{k-j}, T(z)). \end{aligned}$$

We extract the asymptotically relevant terms to obtain

$$W(z)\left(1 - z\sum_{k\in\mathcal{D}} Z(S_{k-1}, T(z))\right) = z^2D(z)T'(z)\sum_{k\in\mathcal{D}} Z(S_{k-2}, T(z)) + O((\rho - z)^{-1}).$$

The right hand side of this equation behaves like $\frac{\rho^2 b}{4}(\rho - z)^{-3/2}$, so this yields

$$W(z) \sim \frac{\rho}{4\alpha}(\rho - z)^{-2}. \quad (18)$$

Thus, if $t_{\mathcal{D},n}$, $d_{\mathcal{D},n}$ and $w_{\mathcal{D},n}$ denote the coefficients of $T(z)$, $D(z)$ and $W(z)$ respectively, we have

$$t_{\mathcal{D},n} \sim \frac{b}{2\sqrt{\pi}}\rho^{-n+1/2}n^{-3/2},\ d_{\mathcal{D},n} \sim \frac{1}{2\alpha}\rho^{-n-1},\ w_{\mathcal{D},n} \sim \frac{1}{4\alpha}\rho^{-n-1}n.$$

So the average values of $D(T_n)$ and $W(T_n)$ for $T_n \in \mathcal{F}_{\mathcal{D}}$ are given by

$$\frac{d_{\mathcal{D},n}}{t_{\mathcal{D},n}} \sim \frac{\sqrt{\pi}}{\alpha b \rho^{3/2}} n^{3/2}, \quad \frac{w_{\mathcal{D},n}}{t_{\mathcal{D},n}} \sim \frac{\sqrt{\pi}}{2\alpha b \rho^{3/2}} n^{5/2},$$

which finally proves the claim. □

In the same manner, we prove our second main theorem:

Theorem 4 *Let $\mathcal{D} \subset \mathbb{N}$ be a subset of the positive integers as in Theorem 1. Then the average Wiener index of a tree $T_n \in \tilde{\mathcal{F}}_{\mathcal{D}}$ is asymptotically $Kn^{5/2}$, where K is defined as in Theorem 1.*

Proof: We use the abbreviations T, D, W again and write $\tilde{T}$, $\tilde{W}$ for $\tilde{T}_{\mathcal{D}}$, $\tilde{W}_{\mathcal{D}}$. We consider the generating function $\tilde{T}(z)$ first:

$$\tilde{T}(z) = z + z \sum_{k \in \mathcal{D}_0} Z(S_{k+1}, T(z)) - \frac{1}{2}\Big(T^2(z) - T(z^2)\Big). \tag{19}$$

Clearly, $\tilde{T}(z)$ must have the same radius of convergence as T, and ρ is the only singularity of $\tilde{T}(z)$ on the circle of convergence. Thus we have to determine the expansion of $\tilde{T}(z)$ around ρ. First, we differentiate (19):

$$\begin{aligned}
\tilde{T}'(z) &= 1 + \sum_{k \in \mathcal{D}_0} Z(S_{k+1}, T(z)) + z \sum_{k \in \mathcal{D}_0} \sum_{l=1}^{k+1} z^{l-1} T'(z^l) Z(S_{k+1-l}, T(z)) - T(z)T'(z) + zT'(z^2) \\
&= 1 + \sum_{k \in \mathcal{D}_0} Z(S_{k+1}, T(z)) + T'(z) \left(z \sum_{k \in \mathcal{D}_0} Z(S_k, T(z)) - T(z) \right) \\
&\quad + z \sum_{k \in \mathcal{D}_0} \sum_{l=2}^{k+1} z^{l-1} T'(z^l) Z(S_{k+1-l}, T(z)) + zT'(z^2) \\
&= 1 + \sum_{k \in \mathcal{D}_0} Z(S_{k+1}, T(z)) + z \sum_{k \in \mathcal{D}} \sum_{l=2}^{k+1} z^{l-1} T'(z^l) Z(S_{k+1-l}, T(z)) + zT'(z^2).
\end{aligned}$$

Thus the derivative of $\tilde{T}(z)$ is bounded at $z = \rho$. Differentiating again yields

$$\tilde{T}''(z) = \sum_{k \in \mathcal{D}_0} T'(z) Z(S_k, T(z)) + z \sum_{k \in \mathcal{D}} \sum_{l=2}^{k+1} z^{l-1} T'(z^l) T'(z) Z(S_{k-l}, T(z)) + \ldots,$$

the remaining terms being bounded at $z = \rho$. We find that

$$\tilde{T}''(z) \sim \left(\beta + \frac{t_0}{\rho}\right) T'(z) = \frac{b^2 \alpha \rho}{2} T'(z)$$

around $z = \rho$. This means that $\tilde{T}(z)$ has an expansion of the form

$$T(z) = \tilde{t}_0 + a_1(\rho - z) + \frac{b^3 \alpha \rho}{3} (\rho - z)^{3/2} + O((\rho - z)^2), \tag{20}$$

giving the asymptotic formula for the number $\tilde{t}_{\mathcal{D},n}$ of trees of size n in $\tilde{F}_{\mathcal{D}}$:

$$t_{\mathcal{D},n} \sim \frac{b^3\alpha}{4\sqrt{\pi}}\rho^{-n+5/2}n^{-5/2}.$$

We only have to determine the expansion of $\tilde{W}(z)$ now. This function is given by $\tilde{W}(z) = \tilde{W}^{(1)}(z) - \tilde{W}^{(2)}(z)$, where $\tilde{W}^{(1)}$ and $\tilde{W}^{(2)}$ are given by (9) and (10) respectively. We extract all asymptotically relevant parts and obtain

$$\begin{aligned}\tilde{W}^{(1)}(z) &= z(D(z)+W(z))\sum_{k\in\tilde{\mathcal{D}}} Z(S_{k-1},T(z)) \\ &\quad + z^2T'(z)(D(z)+zT'(z))\sum_{k\in\tilde{\mathcal{D}}} Z(S_{k-2},T) \\ &\quad + zD(z)\sum_{k\in\tilde{\mathcal{D}}}\sum_{l=2}^{k-1} z^lT'(z^l)Z(S_{k-1-l},T(z)) + O((\rho-z)^{-1/2}) \\ &= z(D(z)+W(z))\sum_{k\in\mathcal{D}_0} Z(S_k,T(z)) \\ &\quad + z^2T'(z)(D(z)+zT'(z))\sum_{k\in\mathcal{D}} Z(S_{k-1},T) \\ &\quad + zD(z)\sum_{k\in\mathcal{D}}\sum_{l=2}^{k} z^lT'(z^l)Z(S_{k-l},T(z)) + O((\rho-z)^{-1/2}).\end{aligned} \tag{21}$$

and

$$\tilde{W}^{(2)}(z) = W(z)T(z) + zT'(z)D(z) + \frac{z^2}{2}T'(z)^2 + O((\rho-z)^{-1/2}). \tag{22}$$

Now, we make use of equations (12) and (13). Some algebraic manipulations then lead us to

$$\begin{aligned}\tilde{W}(z) &= (D(z)+W(z))T(z) - W(z)T(z) + zT'(z)D(z)\left(z\sum_{k\in\mathcal{D}} Z(S_{k-1},T) - 1\right) \\ &\quad + \frac{z^2}{2}T'(z)^2 + z^2T'(z)^2\left(z\sum_{k\in\mathcal{D}} Z(S_{k-1},T) - 1\right) \\ &\quad + zD(z)\sum_{k\in\mathcal{D}}\sum_{l=2}^{k} z^lT'(z^l)Z(S_{k-l},T(z)) + O((\rho-z)^{-1/2}) \\ &= D(z)T(z) + \frac{z^2}{2}T'(z)^2 \\ &\quad - (D(z)+zT'(z))\left(T(z) + z\sum_{k\in\mathcal{D}}\sum_{l=2}^{k} z^lT'(z^l)Z(S_{k-l},T(z))\right) \\ &\quad + zD(z)\cdot\beta + O((\rho-z)^{-1/2}) \\ &= D(z)\cdot t_0 + \frac{z^2}{2}T'(z)^2 - (D(z)+zT'(z))(t_0+\rho\beta) + D(z)\cdot\rho\beta + O((\rho-z)^{-1/2}) \\ &= \frac{z^2}{2}T'(z)^2 + O((\rho-z)^{-1/2}).\end{aligned}$$

Therefore, the expansion of $\tilde{W}$ around ρ is given by

$$\tilde{W}(z) \sim \frac{\rho^2 b^2}{8}(\rho - z)^{-1}, \tag{23}$$

giving us an asymptotic formula for the coefficients of $\tilde{W}(z)$:

$$\tilde{w}_{\mathcal{D},n} \sim \frac{b^2}{8}\rho^{-n+1}.$$

Dividing by $\tilde{t}_{\mathcal{D},n}$ finally yields the theorem. □

As a conclusion, we give numerical values of K for $\mathcal{D} = \{1, \ldots, M\}$ in some special cases:

M	$K(M)$
2	0.7842482154
3	0.6418839467
4	0.5962854459
5	0.5790571390
10	0.5683583008
∞	0.5682799594

Table 3: Some numerical values of K.

Remark: The theorem still holds – mutatis mutandis – when the gcd-condition for $\mathcal{D}$ is violated. In this case, there are several singularities of equal behavior on the circle of convergence. If, for example, $\mathcal{D} = \{3\}$ (in this case, $\tilde{\mathcal{F}}_{\mathcal{D}}$ corresponds to saturated hydrocarbons), there are only trees in $\mathcal{F}_{\mathcal{D}}$ with a number of vertices $n \equiv 1 \mod 3$, and their average Wiener index is asymptotically $0.3705918694 n^{5/2}$.

Remark: It is also possible to determine the moments of the Wiener index of a random tree as well by the same methods. For instance, in the case $\mathcal{D} = \mathbb{N}$, we have

$$\begin{aligned} D(T)^2 &= \left(\sum_{i=1}^{k} D(T_i) + |T| - 1\right)^2 = 2D(T)(|T|-1) - (|T|-1)^2 + \left(\sum_{i=1}^{k} D(T_i)\right)^2 \\ &= 2D(T)(|T|-1) - (|T|-1)^2 + \sum_{i=1}^{k} D(T_i)^2 + \sum_{i \neq j} D(T_i)D(T_j), \end{aligned}$$

which yields the functional equation

$$\begin{aligned} D_2(z) &= 2zD'(z) - 2D(z) - z^2T''(z) + zT'(z) - T(z) \\ &\quad + \left(\sum_{i \geq 1}\sum_{j \geq 1} D(z^i)D(z^j) + \sum_{i \geq 1} iD_2(z^i)\right) T(z) \end{aligned} \tag{24}$$

for the generating function

$$D_2(z) := \sum_T D(T)^2 z^{|T|}.$$

However, the calculations become quite complex and tedious, so we leave out the details of the proof for the sake of brevity. Asymptotic analysis of the functional equations will give the following results:

Theorem 5 *Let T_n be a random rooted tree on n vertices. Then we have, for the variance of $D(T_n)$ and $W(T_n)$ and the covariance of the two,*

$$\begin{aligned}
\mathrm{Var}(D(T_n)) &\sim \frac{10-3\pi}{3\alpha b^2\rho^3} n^3,\\
\mathrm{Cov}(D(T_n), W(T_n)) &\sim \frac{16-5\pi}{10\alpha b^2\rho^3} n^4,\\
\mathrm{Var}(W(T_n)) &\sim \frac{16-5\pi}{20\alpha b^2\rho^3} n^5.
\end{aligned}$$

Also, if $\tilde{T}_n$ is a random tree on n vertices, we have

$$\mathrm{Var}(W(\tilde{T}_n)) \sim \frac{16-5\pi}{20\alpha b^2\rho^3} n^5.$$

Here, $\alpha = 2.95576528\ldots$, $\rho = 0.33832185\ldots$ and $b = 2.68112814\ldots$ as in Theorem 1.

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