On the number of matchings of a tree. *

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Abstract

In a paper of Klazar, several counting examples for rooted plane trees were given, including matchings and maximal matchings. Apart from asymptotical analysis, it was shown how to obtain exact formulas for some of the countings by means of the Lagrange inversion formula. In this note, the results of Klazar are extended to formulas for matchings, maximal matchings and maximum matchings for three types of simply generated trees. Finally, edge coverings are considered and the results are compared.

Key words. Matchings, maximal matchings, edge coverings, simply generated tree, Lagrange inversion

1 Introduction

Enumeration problems for various classes of trees have been in the center of interest of many papers in the past – see for example [10,11,14,16]; among them are rooted plane (ordered) trees, rooted labelled trees, binary (and, generally, s-ary) trees and others. The mentioned classes belong to the so-called simply generated families of trees, whose characteristic analytic property is the fact that the counting series $T(x)$ satisfies a functional equation of the form $T(x) = x\Phi(T(x))$, where $\Phi(t) = \sum_{i=0}^{\infty} c_i t^i$ (the coefficients c_i being non-negative and $c_0 = 1$). Special cases include rooted plane trees ($\Phi(t) = \frac{1}{1-t}$), rooted labelled trees ($\Phi(t) = e^t$; in this case, one works with an exponential generating function) and s-ary trees ($\Phi(t) = (1+t)^s$).

Meir and Moon were able to prove that the coefficients t_n of $T(x)$ follow – under some technical conditions – an asymptotic formula of the type $t_n \sim a\rho^{-n}n^{-3/2}$

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as $n \to \infty$. In a recent paper of Bell, Burris and Yeats [1], this result was extended to a very general theorem about families of rooted trees.

Rooted plane trees have been in the center of interest in a paper of Klazar [11] – he investigates twelve counting problems for rooted plane trees and studies their asymptotic behaviour. Among these are the problems of counting the total number of matchings and maximal matchings in all rooted plane trees of size n.

Klazar describes several applications of the well-known Lagrange inversion formula to his problems; however, he does not give formulas for matchings and maximal matchings. We show how the Lagrange inversion formula is applied to these counting problems and how the hypergeometric summands appearing in the formulas can be interpreted. The version of the Lagrange inversion formula that we will use is the following ([19, p. 99], cf. also [9]):

Theorem 1 (Lagrange inversion formula) *Let $f(x) \in K[[x]]$ be a power series over a field K with $f(0) = 0$, $F(x,y) \in K[[x,y]]$, and suppose that f satisfies the functional equation $f = F(x,f)$. Then for every $k > 0$,*

$$f(x)^k = \sum_{n \geq 1} \frac{k}{n} [y^{n-k}] F(x,y)^n.$$

Here, $[x^n]S(x)$ denotes the coefficient of x^n in the power series $S(x)$.

Furthermore, we will take a look at maximum matchings, which do not appear in the aforementioned paper of Klazar, and compare the results for matchings with those for edge coverings in the final section.

A *matching* is always supposed to mean a set of pairwise disjoint (independent) edges. A k-matching is a matching of exactly k edges. A *maximal matching* is a matching which cannot be expanded by an additional edge. A *maximum matching*, on the other hand, is a matching of largest possible size among all matchings in a graph. For all graph-theoretical notation and terminology, we refer to [5].

2 Matchings

We will consider ordinary matchings first; let $m_1(T,k)$ denote the number of k-matchings of a tree. We derive a functional equation for the generating function

$$M_1(x,y) = \sum_T \sum_{k \geq 0} m_1(T,k) x^{|T|} y^k,$$

where the sum is over all trees T from a simply generated family and $|T|$ denotes the number of vertices. Such a functional equation has already been derived by Klazar in [11] for rooted plane trees. We will repeat his argument and generalize it – we split $M_1(x,y)$ into two parts: $M_1^{(r)}(x,y)$ counting the number of matchings containing the root and $M_1^{(n)}(x,y)$ counting the matchings which do not contain the root. Since a matching of the latter kind simply consists of arbitrary matchings in the subtrees, we obtain

$$M_1^{(n)} = x \sum_{k \geq 0} c_k \left(M_1^{(r)} + M_1^{(n)} \right)^k = x\Phi(M_1^{(r)} + M_1^{(n)}).$$

A matching which contains the root is made up of an edge from the root, a matching which does not contain the root in one of the subtrees and arbitrary matchings in all other subtrees. Therefore, we have

$$M_1^{(r)} = xy \sum_{k \geq 1} k c_k M_1^{(n)} \left(M_1^{(r)} + M_1^{(n)} \right)^{k-1} = xy M_1^{(n)} \Phi'(M_1^{(r)} + M_1^{(n)}).$$

Putting these together yields

$$M_1 = x\Phi(M_1) + x^2 y \Phi(M_1)\Phi'(M_1) = x\left(\Phi(M_1) + xy\Phi(M_1)\Phi'(M_1)\right).$$

We will apply Lagrange inversion to obtain exact expressions for the average number of k-matchings of a tree with n vertices belonging to the family of rooted plane trees ($\Phi(t) = \frac{1}{1-t}$), rooted labelled trees ($\Phi(t) = e^t$) or s-ary trees ($\Phi(t) = (1+t)^s$). The formula for the total number of matchings in all rooted plane trees has already been given by Klazar, but without the combinatorial interpretation for the summands. We start with them for instance: if $\Phi(t) = \frac{1}{1-t}$,

$$\Phi(M_1) + xy\Phi(M_1)\Phi'(M_1) = \frac{1}{1-M_1} + \frac{xy}{(1-M_1)^3},$$

from which the explicit formula for M_1 follows:

$$\begin{aligned} M_1 &= \sum_{l \geq 1} \frac{1}{l} [u^{l-1}] \left(\frac{1}{1-u} + \frac{xy}{(1-u)^3} \right)^l x^l = \sum_{l \geq 1} \frac{1}{l} [u^{l-1}] \sum_{k=0}^{l} \binom{l}{k} \frac{x^k y^k}{(1-u)^{l+2k}} x^l \\ &= \sum_{l \geq 1} \sum_{k=0}^{l} \frac{\binom{l}{k}\binom{2(k+l-1)}{l-1}}{l} x^{k+l} y^k = \sum_{n \geq 1} \sum_{k \leq n/2} \frac{\binom{n-k}{k}\binom{2n-2}{n-k-1}}{n-k} x^n y^k. \end{aligned}$$

If we take into account that the number of rooted plane trees is $\frac{1}{n}\binom{2n-2}{n-1}$, we arrive at our first theorem (the proofs for labelled trees and s-ary trees are similar):

Theorem 2 *The the average number of k-matchings is*

$$\frac{n!(n-1)!}{k!(n+k-1)!(n-2k)!}, \quad \frac{n^{-k} n!}{k!(n-2k)!}, \quad \frac{s^k (sn-k)! n!}{k!(n-2k)!(sn)!}$$

for rooted ordered trees, rooted labelled trees and s-ary trees respectively.

Now, the Stirling formula shows us that the matching sizes asymptotically follow a normal distribution – for rooted plane trees, the average size of a matching is $\mu = \frac{5-\sqrt{13}}{6}$ with a variance of $\sigma^2 = \frac{17\sqrt{13}-52}{117}$. The respective values for rooted labelled trees and s-ary trees are $\mu = \frac{1}{4}$, $\sigma^2 = \frac{1}{12}$ and

$$\mu = \frac{2}{5+\sqrt{\frac{9s-4}{s}}} \text{ and } \sigma^2 = \frac{(10s^2-6s+1)\sqrt{9s^2-4s}-(18s^3-26s^2+8s)}{(4s+1)^2(9s-4)}.$$

It is not a mere coincidence that the coefficients of $M_1(x,y)$ follow a Gaussian distribution – this phenomenon has been studied in a general context by several authors, cf. Bender and Richmond [3], Drmota [6,7], Lalley [13] or Woods [20]. We will use their results in section 4.

As a corollary of Theorem 2, we obtain the average number of *perfect matchings* (i.e. every vertex is incident to an edge of the matching) when we take $k = \frac{n}{2}$. This readily gives us the proportion of trees which have a perfect matching, since perfect matchings of trees are unique (and can be constructed easily by starting from the leaves). The proportion is

$$\frac{n!(n-1)!}{(\frac{n}{2})!(\frac{3n}{2}-1)!} \sim \sqrt{3}\left(\frac{4}{3\sqrt{3}}\right)^n, \quad \frac{n^{-\frac{n}{2}}n!}{(\frac{n}{2})!} \sim \sqrt{2}\left(\frac{2}{e}\right)^{\frac{n}{2}},$$

$$\frac{s^{\frac{n}{2}}((s-\frac{1}{2})n)!\,n!}{(\frac{n}{2})!\,(sn)!} \sim \sqrt{\frac{2s-1}{s}}\left(2\left(1-\frac{1}{2s}\right)^{2s-1}\right)^{\frac{n}{2}}$$

for rooted plane trees, rooted labelled trees and s-ary trees respectively. Their asymptotic number was also studied by Moon in [16] (see also [18]), and explicit formulas were given for rooted plane and rooted labelled trees.

The asymptotic growth of the average total number $a_1(n)$ of matchings has already been given by Klazar in the case of rooted plane trees. His result is easily extended to labelled trees and s-ary trees:

Theorem 3 *The average total number of matchings is of the form $\alpha \cdot \beta^n$ in all three investigated cases, with*

$$\alpha = \sqrt{\frac{65-\sqrt{13}}{78}}, \quad \alpha = \sqrt{\frac{2}{3}}, \alpha = \sqrt{\frac{-1+4s+(4s^2+3s-2)(9s^2-4s)^{-1/2}}{2(1+4s)}}$$

and

$$\beta = \frac{35+13\sqrt{13}}{54}, \ \beta = 2e^{-1/4}, \beta = \frac{\sqrt{9s^2-4s}+s-1}{2s-1} \cdot \left(\frac{8s^2-3s+\sqrt{9s^2-4s}}{8s^2+2s}\right)^s$$

for rooted plane, rooted labelled and s-ary trees respectively.

3 Maximal matchings

Now, we consider maximal matchings, i.e. matchings which cannot be extended any more. We define $m_2(T,k)$ and $M_2(x,y), M_2^{(r)}(x,y), M_2^{(n)}(x,y)$ in the same way as before. The way of reasoning is also the same, and leads to a functional equation for M_2:

$$M_2 = x^2y\Phi(M_2)\Phi'(M_2) + x\Phi(x^2y\Phi(M_2)\Phi'(M_2)).$$

Now, we determine an exact formula for the total number of maximal matchings in rooted plane trees. In this case, we have

$$xy\Phi(M_2)\Phi'(M_2) + \Phi(x^2y\Phi(M_2)\Phi'(M_2)) = \frac{xy}{(1-M_2)^3} + \frac{1}{1-\frac{x^2y}{(1-M_2)^3}}.$$

Now, the Lagrange inversion formula shows that

$$\begin{aligned}
M_2 &= \sum_{l\geq 1}\frac{1}{l}[u^{l-1}]\left(\frac{xy}{(1-u)^3}+\frac{1}{1-\frac{x^2y}{(1-u)^3}}\right)^l x^l \\
&= \sum_{l\geq 1}\frac{1}{l}[u^{l-1}]\sum_{m=0}^{l}\binom{l}{m}\left(\frac{xy}{(1-u)^3}\right)^{l-m}\left(1-\frac{x^2y}{(1-u)^3}\right)^{-m} x^l \\
&= \sum_{l\geq 1}\frac{1}{l}[u^{l-1}]\sum_{m=0}^{l}\binom{l}{m}x^{2l-m}y^{l-m}(1-u)^{-3l+3m}\sum_{r\geq 0}(-1)^r\binom{-m}{r}\left(\frac{x^2y}{(1-u)^3}\right)^r \\
&= \sum_{l\geq 1}\sum_{m=0}^{l}\sum_{r\geq 0}\frac{1}{l}\binom{l}{m}\binom{m+r-1}{r}\binom{4l-3m+3r-2}{l-1}y^{l+r-m}x^{2l+2r-m}.
\end{aligned}$$

Next, we perform a change of variables: we set $2l+2r-m = n$ and $l+r-m = k$. Then $m = n-2k$ and $r = n-k-l$, so that we obtain

$$M_2 = \sum_{n\geq 1}\sum_{k\leq n/2}\sum_{l=\max(n-2k,1)}^{n-k}\frac{1}{l}\binom{l}{n-2k}\binom{2n-3k-l-1}{n-k-l}\binom{3k+l-2}{l-1}x^ny^k.$$

If $n = 2k$, then the inner sum is given by $\sum_{l=1}^{k}\frac{1}{l}\binom{k-l-1}{k-l}\binom{3k+l-2}{l-1}$. But $\binom{k-l-1}{k-l}$ equals 0 unless $l = k$, so the sum is $\frac{1}{k}\binom{4k-2}{k-1}$ in this case. If $n \neq 2k$, we set $a = n-2k$ and $b = n-k$ ($k = b-a$). Then the inner sum can be rewritten as

$$\frac{(3b-2a-2)!}{a!(3b-3a-1)!}\sum_{l=a}^{b}\binom{a+b-l-1}{b-l}\binom{3b-3a+l-2}{l-a} = \frac{(3b-2a-2)!\binom{4b-2a-2}{b-a}}{a!(3b-3a-1)!},$$

where the latter equality follows from Vandermonde's convolution formula (see [9]). Rewriting in terms of n and k gives $\frac{1}{3k-1}\binom{n+k-2}{n-2k}\binom{2n-2}{k}$, which is also the correct result in the case $n = 2k$. Similar calculations can be performed for rooted labelled trees and s-ary trees, yielding the following theorem:

Theorem 4 *The average number of maximal matchings of size k is*

$$\frac{n!(n-1)!(n+k-2)!}{k!(3k-1)!(n-2k)!(2n-k-2)!}, \quad \frac{n^{k-n+1}(2k)^{n-2k-1}n!}{k!(n-2k)!},$$

$$\frac{s^k((2s-1)k)!((s-1)n+k+1)!n!}{k!(n-2k)!(sn)!((2s+1)k-n+1)!}$$

for rooted ordered, rooted labelled and s-ary trees respectively.

Note also that a maximal matching must comprise at least $\frac{1}{2s+1}$ of the edges of an s-ary tree.

The asymptotics of the average total number $a_2(n)$ of maximal matchings were given by Klazar in the case of rooted plane trees. We extend it to the following theorem (here and in the following, we give all numerical values to a precision of six digits after the decimal point):

Theorem 5 *The average total number of maximal matchings is of the form $\alpha \cdot \beta^n$ in all three investigated cases, with $\alpha = 0.856092,\ 0.797079,\ 0.762502$ and $\beta = 1.305398,\ 1.313080,\ 1.317840$ for rooted plane, rooted labelled and binary trees respectively.*

REMARK: Again, the sizes follow a normal distribution – the mean values and variances are $\mu = 0.320640,\ 0.357045,\ 0.381260$ and $\sigma^2 = 0.042618,\ 0.033072,\ 0.026002$ for rooted plane, rooted labelled and binary trees respectively. We conclude with a corollary on the proportion of maximal matchings among k-matchings:

Corollary 6 The proportion of maximal matchings among all k-matchings is given by

$$\frac{(n+k-1)!(n+k-2)!}{(3k-1)!(2n-k-2)!}, \quad \left(\frac{2k}{n}\right)^{n-2k-1}, \quad \frac{((2s-1)k)!((s-1)n+k+1)!}{((2s+1)k-n+1)!(sn-k)!}$$

for rooted plane trees, rooted labelled trees and s-ary trees respectively. All these expressions are strictly increasing in k and attain 1 at $k = \lfloor \frac{n}{2} \rfloor$.

4 Maximum matchings

We turn to maximum matchings now, i.e. matchings of maximal possible size. Every maximum matching is maximal, but not vice versa. First of all, we divide the set of rooted trees into two subsets:

- The set of rooted trees which have a maximum matching not containing an edge incident to the root.
- The set of rooted trees which do not have such a matching.

It is easy to see that a rooted tree belongs to the first set if and only if each of its subtrees belongs to the second set. Therefore, if $A(x)$ and $B(x)$ denote the generating functions for the number of trees from a fixed simply generated family which belong to the first and second set respectively, we have

$$A = x\Phi(B),\ B = x\Phi(A+B) - x\Phi(B).$$

The two classes correspond exactly with the *losing* and *winning* trees from [17], where it is shown that the ratio between the two classes tends to a constant as the number of vertices goes to infinity. If, for instance, $\Phi(t) = e^t$, we obtain $A = x\exp\Big(A(e^A - 1)\Big)$. Application of the Lagrange inversion formula now shows that

$$A = \sum_{k\geq 1} \frac{k^{k-2}}{(k-1)!} \sum_{r=0}^{k-1} \binom{k-1}{r} \left(-\frac{r+1}{k}\right)^r x^k.$$

Similar formulas can be given for rooted labelled trees and s-ary trees. We also note that $A(x) = W(-W(-x))$, and $B(x) = -W(-x) - A(x)$, where $W(x)$ is *Lambert's W-function*, defined as the solution of $we^w = x$. A simple application of the Flajolet-Odlyzko singularity analysis (s. [8]) now shows that the quotient of the number of trees of the first type and the number of trees of the second type is asymptotically $\Omega = W(1) = 0.567143$, which is also called the *omega constant*. The omega constant is an exponential golden ratio in a certain sense, so it is interesting to see that we obtain a quotient of ϕ^2 (where $\phi = \frac{\sqrt{5}-1}{2}$ is the golden ratio) for rooted plane trees. For $\Phi(t) = (1+t)^s$, the quotient tends to $\frac{s\alpha}{s-\alpha}$, where α is a solution of $\alpha = \left(1 - \frac{\alpha}{s}\right)^s$.

The classification of trees in two categories will help us to count the number of maximum matchings now. We need four auxiliary functions:

- $A_1(x,y)$ and $A_2(x,y)$ count the number of maximum matchings which contain resp. don't contain the root, summed over all trees of the first category.
- $B_1(x,y)$ and $B_2(x,y)$ count the number of largest possible matchings which contain resp. don't contain the root, summed over all trees of the second category (they are maximum matchings if they contain the root).

The generating function for the total number of maximum matchings is given by $M_3(x,y) = A_1(x,y)+A_2(x,y)+B_1(x,y)$. We determine functional equations for our functions in the same way as in the previous sections:

$$A_1 = xyB_2\Phi'(B_1),\ A_2 = x\Phi(B_1),\ B_1 = xyA_2\Phi'(M_3),\ B_2 = x(\Phi(M_3)-\Phi(B_1)).$$

The Lagrange inversion formula doesn't give us nice results any more for this system; therefore, we will only be concerned with the asymptotical behaviour.

For this purpose, we will use the Drmota-Lalley-Woods theorem [6], which deals with systems of equations of the general type $\mathbf{z} = \mathbf{F}(x, \mathbf{y}, \mathbf{z})$, where $\mathbf{z}$ is a vector of functions in x and $\mathbf{y}$ and $\mathbf{F}$ is a vector of analytic functions: if $x = x(\mathbf{y})$ and $\mathbf{z} = \mathbf{z}(\mathbf{y})$ are solutions of the system

$$\mathbf{z} = \mathbf{F}(x, \mathbf{y}, \mathbf{z}),\ 0 = \det(\mathbf{I} - \mathbf{F}_{\mathbf{z}}(x, \mathbf{y}, \mathbf{z})),$$

$\mu = -\frac{x_{\mathbf{y}}(\mathbf{1})}{x(\mathbf{1})}$ and $\sigma^2 = -\frac{x_{\mathbf{y}\mathbf{y}}(\mathbf{1})}{x(\mathbf{1})} + \mu^T\mu + \mathrm{diag}(\mu)$, then – under some regularity conditions which are satisfied in our case – the coefficients of $[x^n]z_j$ asymptotically follow a Gaussian distribution: if

$$z_j = \sum_{n,\mathbf{m}} z_{j,n,\mathbf{m}} x^n \mathbf{y}^{\mathbf{m}}$$

and $z_{j,n} = \sum_{\mathbf{m}} z_{j,n,\mathbf{m}}$, the random variable $\mathbf{X}_n$ with $P(\mathbf{X}_n = \mathbf{m}) = \frac{z_{j,n,\mathbf{m}}}{z_{j,n}}$ is asymptotically normal with mean μn and covariance matrix $\sigma^2 n$. Furthermore, $z_{j,n} \sim a_j x(\mathbf{1})^{-n}$ for constants a_j which can be determined by Bender's formula (in its corrected form due to Canfield, Meir and Moon [4,15]) as was described in the paper of Klazar. We will skip the details of the calculation (which merely involve the numerical solution of systems of equations), but only give the numerical values for rooted plane trees, rooted labelled trees and binary trees: in all cases, the average total number of maximum matchings is $a_3(n) \sim \alpha \cdot \beta^n$, the sizes are normally distributed with mean μ and variance σ^2.

- r. plane trees: $\alpha = 0.935963$, $\beta = 1.216646$, $\mu = 0.344786$, $\sigma^2 = 0.040908$.
- r. labelled trees: $\alpha = 0.982760$, $\beta = 1.187581$, $\mu = 0.395787$, $\sigma^2 = 0.025496$.
- binary trees: $\alpha = 1.154412$, $\beta = 1.153092$, $\mu = 0.433982$, $\sigma^2 = 0.013519$.

5 Edge coverings

In this final chapter, we will consider edge coverings. An edge covering of a graph G is a set $U \subseteq V(G)$ of vertices with the property that every edge of G has an end in U. Our motivation for comparing edge coverings with matchings is the celebrated theorem of König (see [5]):

Theorem 7 (König) *The largest size of a matching in a bipartite graph G equals the smallest size of an edge covering in G.*

It is easy to see that a set U is an edge covering if and only if the complementary set $V(G) \setminus U$ is independent, so there is a bijective correspondence between independent sets and edge coverings. Since independent and maximal independent sets have already been examined by Kirschenhofer, Prodinger and Tichy [10], Meir and Moon [14] and Klazar [11], we will not investigate them any further. For the sake of completeness, we give the asymptotics for the average numbers $e_1(n)$, $e_2(n)$ of edge coverings resp. minimal edge coverings in three cases:

- r. plane trees: $(1.026400) \cdot (1.687500)^n$ resp. $(1.060528) \cdot (1.239369)^n$.
- r. labelled trees: $(1.091139) \cdot (1.655488)^n$ resp. $(1.022451) \cdot (1.273865)^n$.
- binary trees: $(1.129277) \cdot (1.637420)^n$ resp. $(0.994709) \cdot (1.296596)^n$.

Finally, we consider minimum edge coverings. It seems logical to divide the family of rooted trees into two classes – those with a minimum edge covering containing the root and those with no such edge covering. However, we do not need to count these classes any more, since they correspond exactly to the classes defined for maximum matchings. This is due to the following fact, which is an immediate consequence of König's theorem:

Theorem 8 *Let G be a bipartite graph and $v \in V(G)$. If every maximum matching of G contains an edge incident with v, then there exists a minimum edge covering of G which contains v and vice versa.*

Now, we can proceed exactly as in the previous section and obtain the following numerical results for the average total number of minimum edge coverings $e_3(n) \sim \alpha \cdot \beta^n$ and the distribution of sizes:

- r. plane trees: $\alpha = 1.042383$, $\beta = 1.132343$, $\mu = 0.417680$, $\sigma^2 = 0.042029$.
- r. labelled trees: $\alpha = 1.093753$, $\beta = 1.140355$, $\mu = 0.459106$, $\sigma^2 = 0.019952$.
- binary trees: $\alpha = 1.248636$, $\beta = 1.129720$, $\mu = 0.482126$, $\sigma^2 = 0.008294$.

We see that, interestingly, the average number of edge coverings is asymptotically larger than the average number of matchings, whereas the number of minimal/minimum edge coverings is asymptotically smaller than the respective number for matchings.

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