ASYMPTOTIC DISTRIBUTIONS AND A MULTIVARIATE DARBOUX METHOD IN ENUMERATION PROBLEMS

Michael Drmota

Technical University of Vienna

Abstract. Let $c(x,z) = \sum c_{nk} x^n z^k$ ($c_{nk} \ge 0$) be a bivariate generating function satisfying a functional equation $c = G(c,x,z)$. By using a central limit theorem of E.A. Bender it is shown that discrete random variables X_n with $P[X_n = k] = c_{nk}/(\sum c_{ni})$ are asymptotically normal with mean $\mu_n \sim \mu n$ and variance $\sigma_n^2 \sim \sigma^2 n$. Furthermore a bivariate asymptotic expansion for the coefficients c_{nk} can be obtained by two different methods. After some applications to tree enumeration problems a multivariate Darboux-method is formulated.

1. Introduction

Many enumeration problems can be treated by using generating functions. But there are only few cases where it is possible to obtain explicit expressions for the coefficients. So it is often very useful to know something about the asymptotic behaviour.

For example consider the case of independent subsets of trees in a simply generated family of trees ([KPT]). (A subset I of nodes of a graph is called independent if no two nodes of I are joined to each other.) Let c_{nk} be the total number of independent subsets of size k in trees of size n (contained in a simply generated family of trees). Then the generating function $c(x,z) = \sum c_{nk} x^n z^k$ satisfies

$$c = xz\varphi(x\varphi(c)) + x\varphi(c), \tag{1.1}$$

where $\varphi(t) = 1 + \varphi_1 t + \cdots$ characterizes the family of trees. In general it is not possible to get an explicit formula for c_{nk} but if $\varphi(t) = 1/(1-t)$ (that is the case of general planted plane trees) it is shown in [KPT] by using Lagrange's inversion formula that

$$c_{nk} = \frac{2}{n}\binom{n}{k}\binom{2n-3}{n-k-1} \tag{1.2}$$

and

$$c_n = \sum_{k=0}^{n} c_{nk} = \frac{2}{n}\binom{3n-3}{n-1}. \tag{1.3}$$

Therefore independent subsets of size k of general planted plane trees of size n are hypergeometrically distributed with mean

$$\mu_n = \frac{1}{c_n}\sum_{k=0}^{n} k\, c_{nk} = \frac{n}{3} \tag{1.4}$$

and variance
$$\sigma_n^2 = \frac{1}{c_n}\sum_{k=0}^{n}(k-\mu_n)^2 c_{nk} = \frac{2n(2n-3)}{9(3n-4)}. \tag{1.5}$$
So they are asymptotically normal and in addition asymptotic expansions for c_{nk} can easily be obtained by Stirling's formula.

But as mentioned before the simplicity of this example is not the rule. Explicit formulas are very rare and even if they exist they are often useless for practical calculations (see section 4).

So the object of this paper is to discuss the asymptotic behaviour of c_{nk} if $c(x,z) = \sum c_{nk}x^n z^k$ satisfies a functional equation of type
$$c = G(c,x,z). \tag{1.6}$$
In fact it will be proved by two different methods (one by E.A. Bender [B], [BR] in section 2, the other motivated by P. Kirschenhofer [K1], [K2] in section 3) that under some weak conditions on $G(c,x,z)$ discrete random variables X_n with $P[X_n = k] = c_{nk}/\left(\sum c_{ni}\right)$ are asymptotically normal and that bivariate asymptotic expansions for c_{nk} can be obtained. In section 4 we will apply these results to independent and maximal independent subsets of trees and in section 5 we will formulate a multivariate Darboux method based on a theorem of E.A. Bender and L.B. Richmond [BR].

2. Bender's method

The basic tool is the following theorem of E.A. Bender [BR]:

Theorem 1. *Let $c(x,z) = \sum c_{nk}x^n z^k$ be a generating function of non-negative numbers c_{nk} that has positive radius of convergence (as a function in x) if $z = 1+\varepsilon$ for some $\varepsilon > 0$. Suppose that*
$$\varphi_n(z) = \sum_k c_{nk}z^k \sim a_n g(z)\lambda(z)^n \quad (n\to\infty) \tag{2.1}$$
uniformly in $K(1,\varepsilon) = \{z : |z-1| < \varepsilon\}$, where $a_n > 0$, $g(z)$ is uniformly continuous and $\lambda(z)$ has quadratic Taylor series expansion with error term $O(|z-1|^3)$. If $\frac{d^2}{ds^2}\log\lambda(e^s)|_{s=0} \neq 0$ then discrete random variables X_n with $P[X_n = k] = c_{nk}/c_n$ $(c_n = \varphi_n(1))$ are asymptotically normal with mean
$$\mu_n = EX_n = \frac{1}{c_n}\sum_{k=0}^{n} k\,c_{nk} \sim \mu\, n \quad (n\to\infty) \tag{2.2}$$
and variance
$$\sigma_n^2 = VX_n = \frac{1}{c_n}\sum_{k=0}^{n}(k-\mu_n)^2 c_{nk} \sim \sigma^2\, n, \quad (n\to\infty) \tag{2.3}$$
where
$$\mu = \frac{d}{ds}\log\lambda(e^s)|_{s=0} \quad \textit{and} \quad \sigma^2 = \frac{d^2}{ds^2}\log\lambda(e^s)|_{s=0}. \tag{2.4}$$

Sketch of proof. Notice that the characteristic function of
$Y_n = (X_n - \mu_n)/\sigma_n$ which is given by

$$\Phi_{Y_n}(t) = e^{-i\mu_n t/\sigma_n}\varphi_n\left(e^{it/\sigma_n}\right)/\varphi_n(1) \tag{2.5}$$

converges to $e^{-t^2/2}$.

Under some additional conditions it is also possible to get an asymptotic expansion for c_{nk}. The following theorem is a combination of the results of [B] (especially Theorem 3) and of [BR]:

Theorem 2. *Let $c(x,z) = \sum c_{nk}x^n z^k$ be a generating function of non-negative numbers c_{nk} and let $a < b$ be positive real numbers such that $c(x, b+\varepsilon)$ has positive radius of convergence (as a function in x) for some $\varepsilon > 0$. Suppose that (2.1) holds uniformly in $R(a,b,\phi) = \{z : a \le |z| \le b, |arg(z)| \le \phi\}$ for some $\phi > 0$, where $a_n > 0$, $g(z)$ is continuous and non-zero and $\lambda(z)$ is non-zero and has bounded third derivative for $z \in R(a,b,\phi)$. Furthermore suppose that $\frac{d^2}{ds^2}\log\lambda(e^s)|_{e^s=z} \ne 0$ for $z \in [a,b]$ and that there exists a $\delta > 0$ such that $c(x,z)$ is analytic and bounded for $|z| \in [a,b]$, $z \notin R(a,b,\phi)$, and $|x| \le (1+\delta)/\lambda(|z|)$. Then $\frac{d^2}{ds^2}\log\lambda(e^s)|_{e^s=z} > 0$ and we have*

$$c_{nk} \sim \frac{a_n}{\sqrt{2\pi n}}\frac{g\left(h\left(\frac{k}{n}\right)\right)}{\sigma\left(h\left(\frac{k}{n}\right)\right)}\frac{\lambda\left(h\left(\frac{k}{n}\right)\right)^n}{h\left(\frac{k}{n}\right)^k} \tag{2.6}$$

uniformly for $k/n \in [\mu(a), \mu(b)]$, where

$$\mu(z) = \frac{d}{ds}\log\lambda(e^s)|_{e^s=z}, \tag{2.7}$$

$$\sigma(z) = \left(\frac{d^2}{ds^2}\log\lambda(e^s)|_{e^s=z}\right)^{1/2}, \tag{2.8}$$

and $h(t)$ is the inverse function of $\mu(z)$.

Now we will apply this theorem to generating functions $c(x,z)$ which satisfy a functional equation of the form $c = G(c,x,z)$.

Theorem 3. *Let $c(x,z) = \sum c_{nk}x^n z^k = \sum \varphi_n(z)x^n$ be a generating function of non-negative numbers c_{nk} such that there are n_1, n_2, n_3, $k_1 < k_2 < k_3$ with $c_{n_1k_1}c_{n_2k_2}c_{n_3k_3} > 0$ and $gcd(k_3-k_1, k_2-k_1) = 1$. Set $d = gcd\{n - l : \varphi_n(z) \ne 0\}$, where $l = \min\{m > 0 : \varphi_m(z) \ne 0\}$. Furthermore let $c(x,z)$ satisfy a functional equation $c = G(c,x,z)$, where the expansion $G(c,x,z) = \sum g_{ijk}c^i x^j z^k$ has non-negative coefficients g_{ijk} and suppose that the system of equations*

$$\begin{aligned} c &= G(c,x,z) \\ 1 &= G_c(c,x,z) \end{aligned} \tag{2.9}$$

has positive solutions $c = f_1(z)$, $x = f_2(z)$ for $z \in [a,b]$ such that $(f_1(z), f_2(z), z)$ are regular points of the series expansion of $G(c,x,z)$. (If there is more than one solution, $x = f_2(z)$ should be chosen minimal.) In addition suppose that

$$G_x(f_1(z), f_2(z), z)\cdot G_{cc}(f_1(z), f_2(z), z) > 0 \tag{2.10}$$

and that

$$\begin{aligned}\sigma(z)^2 = \Bigg[&\left(\frac{zG_z}{xG_x}\right)^2 + \frac{zG_z}{xG_x} \\ &+ \frac{z^2}{xG_x^3 G_{cc}} \Big(G_x^2 (G_{cc}G_{zz} - G_{cz}^2) - 2G_x G_z (G_{cc}G_{xz} - G_{cx}G_{cz}) \\ &\quad + G_z^2 (G_{cc}G_{xx} - G_{cx}^2) \Big) \Bigg] (f_1(z), f_2(z), z) \\ \neq 0. \end{aligned} \tag{2.11}$$

Then $\sigma(z)^2 > 0$ *and we have*

$$c_{nk} = \frac{d}{2\pi n^2} \frac{g\left(h\left(\frac{k}{n}\right)\right)}{\sigma\left(h\left(\frac{k}{n}\right)\right)} \frac{1}{h\left(\frac{k}{n}\right)^k \; f_2\left(h\left(\frac{k}{n}\right)\right)^n} \left(1 + O\left(n^{-1/2}\right)\right) \tag{2.12}$$

uniformly for $k/n \in [\mu(a), \mu(b)]$ *and* $n \equiv l \mod d$, *where*

$$g(z) = \left(\left[\frac{xG_x}{G_{cc}} \right] (f_1(z), f_2(z), z) \right)^{1/2}, \tag{2.13}$$

$$\mu(z) = \left[\frac{zG_z}{xG_x} \right] (f_1(z), f_2(z), z), \tag{2.14}$$

and $h(t)$ *is the inverse function of* $\mu(z)$.

If $1 \in (a,b)$ *then discrete random variables* X_n *with* $P[X_n = k] = c_{nk}/c_n$ $(n \equiv l \mod d)$ *are asymptotically normal with mean* $\mu_n = EX_n$ *and variance* $\sigma_n^2 = VX_n$. *They can be determined asymptotically by*

$$\begin{aligned} \mu_n &= \mu(1)\, n + O(1), \\ \sigma_n^2 &= \sigma(1)^2\, n + O(1). \end{aligned} \qquad (n \to \infty) \tag{2.15}$$

$c_n = \varphi_n(1)$ *has the asymptotic expansion*

$$c_n = \frac{d}{\sqrt{2\pi}}\, g(1)\, f_2(1)^{-n}\, n^{-3/2} \left(1 + O\left(n^{-1}\right)\right), \quad (n \to \infty) \tag{2.16}$$

Remark 1. The gcd-condition on the coefficients c_{nk} is equivalent to $|G_c(c(x,z),x,z)| < G_c(c(|x|,|z|),|x|,|z|)$ for $z \neq |z|$. Therefore it is sufficient to guarantee only this property. (This can be seen similarly to [MM2].)

Remark 2. It may happen that the expansion of $G(c,x,z)$ has not only non-negative coefficients but it is possible to introduce a new variable d such that

$$\begin{aligned} d &= H(d,x,z) \\ c &= F(c,x,z), \end{aligned} \tag{2.17}$$

where the coefficients h_{ijk} of the expansion $H(d,x,z) = \sum h_{ijk} d^i x^j z^k$ are non-negative and H and F are regular at the solutions of $d = H(c,x,z)$, $1 = H_d(d,x,z)$. Then Theorem 3 remains true.

Remark 3. Sometimes it may occur that $f_1(z)$ or $f_2(z)$ cannot be calculated explicitely but the system of equations

$$\begin{aligned} c &= G(c,x,z) \\ 1 &= G_c(c,x,z) \\ z\,G_z(c,x,z) &= \rho\, x\, G_x(c,x,z) \end{aligned} \tag{2.18}$$

has explicit posive solutions (c_ρ, x_ρ, z_ρ) for $\rho \in [\alpha,\beta]$. ($x_\rho > 0$ should be chosen minimal.) Then $c_\rho = f_1(h(\rho))$, $x_\rho = f_2(h(\rho))$, $z_\rho = h(\rho)$, and we get an explicit asymptotic expansion.

$$c_{nk} = \frac{d}{2\pi n^2}\frac{g(z_{k/n})}{\sigma(z_{k/n})}\, z_{k/n}^{-k}\, x_{k/n}^{-n}\left(1 + O\left(n^{-1/2}\right)\right) \tag{2.19}$$

uniformly for $k/n \in [\alpha,\beta]$ and $n \equiv l \mod d$. Note that $\mu(z_\rho) = \rho = -(z_\rho \frac{d}{d\rho}x_\rho)/(x_\rho \frac{d}{d\rho}z_\rho)$ and that this implies that $\sigma^2(z_\rho)$ can be evaluated by $z_\rho/\frac{d}{d\rho}z_\rho$.

Remark 4. If the distributions are asymptotically normal it is possible to get asymptotic expansions for higher centralized moments

$$\mu_c^{(l)} = \frac{1}{c_n}\sum_k (k-\mu_n)^l c_{nk}, \tag{2.20}$$

too. We have

$$\mu_c^{(2s)} = \frac{2^s\sigma(1)^{2s}}{\sqrt{\pi}}\,\Gamma(s+1/2)\, n^s + O\left(n^{s-1}\right) \tag{2.21}$$

and

$$\mu_c^{(2s+1)} = O\left(n^s\right). \tag{2.22}$$

Proof of Theorem 3. Since $c(x,z)$ is the solution of $c = G(c,x,z)$ it can be analytically continued as long as $G_c(c(c,z),x,z) \neq 1$ by the implicit function theorem. If $z > 0$ is fixed the radius of convergence of $c(x,z)$ is the first singularity on the positive real axis since the coefficients of $c(x,z)$ are non-negative. Furthermore this singularity $x = f_2(z)$ can be obtained by solving the system of equations (2.9) for $z \in [a,b]$ $(0 < a < b)$. The solution $c = f_1(z) > 0$, $x = f_2(z) > 0$ must be chosen in a way that $f_2(z) > 0$ is minimal. In addition one obtains (see [MM2]) that the series expansion of $c(x,z)$ converges at $x = f_2(z)$ and $c(f_2(z),z) = f_1(z)$. Again by the implicit function theorem and (2.10) the functions $f_1(z)$, $f_2(z)$ can be continued analytically to some neighbourhood of $R(a,b,\phi)$. So we have an expansion of the following form:

$$\begin{aligned} c(x,z) = f_1(z) - \left[\frac{2\,G_x(f_1(z),f_2(z),z)}{G_{cc}(f_1(z),f_2(z),z)}\right]^{1/2} &\sqrt{f_2(z)-x}\,\cdot \\ &\cdot (1 + (f_2(z)-x)h_1(x,z)) \\ + (f_2(z)-x)h_2(x,z) & \end{aligned} \tag{2.23}$$

for $z \in R(a,b,\phi)$ and x in some neighbourhood of $f_2(z)$ where the cut $\arg(f_2(z) - x) = \pi$ is excluded. $h_1(x,z)$ and $h_2(x,z)$ are analytic functions for $z \in R(a,b,\phi)$

and and x in some neighbourhood of $f(z)$. Since $c(\zeta_d x,z)=\zeta_d^l c(x,z)$, where ζ_d is a d-th root of unity and $l=\min\{m>0:\varphi_m(z)\neq 0\}$ we have similar expansions for x in some neighbourhood of $\zeta_d f_2(z)$. So we get by Darboux's theorem that

$$\varphi_n(z)=\frac{d}{2\sqrt{\pi}}\left[\frac{2f_2(z)G_x(f_1(z),f_2(z),z)}{G_{cc}(f_1(z),f_2(z),z)}\right]^{1/2} f_2(z)^{-n}\,n^{-3/2}\cdot \left(1+O\left(n^{-1}\right)\right) \tag{2.24}$$

uniformly in $R(a,b,\phi)$ for $n\equiv l \mod d$ and there are no other singularities on the cirlce of convergence $|x|=f_2(z)$ for $z\in[a,b]$. The gcd-condition implies that $|G_c(c(x,z),x,z)|<G_c(c(|x|,|z|),|x|,|z|)$ for $z\neq|z|$. So $c(x,z)$ can be analytically continued from $|z|\in[a,b]$, $z\notin R(a,b,\phi)$, $|x|\le f_2(|z|)$ to some region $|x|\le f_2(|z|)(1+\delta)$, where $\delta>0$ can be chosen independently for $|z|\in[a,b]$, $z\notin R(a,b,\phi)$. This implies that $c(x,z)$ is analytic and bounded for $|z|\in[a,b]$, $z\notin R(a,b,\phi)$, and $|x|\le f_2(|z|)(1+\delta)$. So Theorem 1 and 2 apply. The error term of the bivariate asymptotic expansion (2.12) can be obtained by examining the proof of [B, Theorem 3]. The asymptotic expansion (2.16) is a direct consequence of (2.24). In order to get the error terms in (2.15), (2.21), and (2.22) notice that

$$\begin{aligned}\sum_n \mu_n c_n x^n &= c_z(x,1)\\ &=\frac{G_z(c(x,1),x,1)}{G_x(c(x,1),x,1)}\,c_x(x,1)\\ &=\left[\frac{G_z}{G_x}\left(\frac{2G_x}{G_{cc}}\right)^{1/2}\right](f_1(1),f_2(1),1)\frac{1}{\sqrt{f_2(1)-x}}+\cdots.\end{aligned} \tag{2.25}$$

So by Darboux's theorem and (2.16) we have

$$\mu_n=\left[\frac{G_z}{xG_x}\right](f_1(1),f_2(1),1)\,n+O(1). \tag{2.26}$$

Similarly we can argue for σ_n^2 and $\mu_c^{(l)}$.

3. Kirschenhofer's method

The basic tool of this second method is the following Lemma (see [K1], [K2]).

Lemma 1. *Let $0<\rho=p/r\in\mathbf{Q}$ with $gcd(p,r)=1$. Then*

$$d_\rho(t)=\sum_l c_{rl,pl}\,t^{rl}=\frac{1}{2\pi i}\int_{\mathcal{C}(t)} c\left(\frac{t}{s^p},s^r\right)\frac{ds}{s}, \tag{3.1}$$

where $\mathcal{C}(t)$ is a positively oriented simple closed curve separating all singularities of $b_t(s)=c(t/s^p,s^r)$ which tend to zero for t tending to zero from the others. Furthermore non-polar singularities tending to zero must be separated from one another.

Remark 5. Lemma 1 must be interpreted in the following way. If $|t|<z^\rho f_2(z)$ for some $z\in[a,b]$ it is possible to find a circle $\mathcal{C}(t)=\{s:\,|s|=R\}$ with $(|t|/f_2(z))^{1/p}<$

$R < z^{1/r}$ so that $|t|/R^p < f_2(z)$ and $R^r < z$. Thus $b_t(s)$ is analytic around $\mathcal{C}(t)$ and it is easy to see that (3.1) holds in this case. Furthermore $\mathcal{C}(t)$ separates the singularities tending to zero from the others. Therefore $d_\rho(t)$ can be analytically continued by the integral representation (3.1). This will be used to find the type of singularity of $d_\rho(t)$ at the radius of convergence.

For brevity we will only sketch the ideas of this method and only discuss the case $d = 1$. In order to reach uniformity for $\rho \in [\alpha, \beta]$ we will proceed as follows. For every fixed $\rho \in [\alpha, \beta]$ it will be shown that there is a neighbourhood $U(\rho)$ of ρ such that all estimates are uniform in $U(\rho)$. So we are done by the compactness of $[\alpha, \beta]$.

Using the implicit function theorem and (2.10) it can be shown that for $t = t_\rho = x_\rho z_\rho^\rho$, where (c_ρ, x_ρ, z_ρ) is the solution of (2.18), there are locally two algebraic singularities $s_1(t) < s_2(t)$ with expansions (compare with [Dr])

$$\begin{aligned} s_1(t) &= s_\rho - u_0\sqrt{t_\rho - t}\,(t + (t_\rho - t)u_1(t)) + (t_\rho - t)u_2(t) \\ s_2(t) &= s_\rho + u_0\sqrt{t_\rho - t}\,(t + (t_\rho - t)u_1(t)) + (t_\rho - t)u_2(t), \end{aligned} \tag{3.2}$$

where $s_\rho = z_\rho^{1/r}$, $s_1(t)$ is a singularity tending to zero for t tending to zero, and $s_2(t)$ is not of this kind. Therefore $d_\rho(t)$ is analytic for $|t| < t_\rho$ and for $|t| < t_\rho(1+\gamma_\rho)$, $\arg(t) \ne 2\pi j/r$ $(j = 1, 2, \ldots, r)$ for some $\gamma_\rho > 0$ since it is possible to choose a proper contour $\mathcal{C}(t)$. Note that $d_\rho\left(te^{2\pi i j/r}\right) = d_\rho(t)$. So one might expect that t_ρ is the radius of convergence of $d_\rho(t)$.

$d = 1$ and the gcd-condition imply that it is possible to find a circle $\mathcal{C} = \mathcal{C}(t) = \{s : |s| = R_\rho\}$ such that $c(t/s^p, s^r)$ is analytic and bounded for $|t| = t_\rho(1+\gamma_\rho)$, $\max_j(\arg(t) - 2\pi j/r) > \phi$ and $s \in \mathcal{C}$. Furthermore there is a neighbourhood $U(\rho)$ of ρ such that this bound is uniform for all rationals in $U(\rho)$. (R_ρ must be chosen such that $R_\rho^{1/r} = \text{const.}$.) Since $d_\rho\left(te^{2\pi i j/r}\right) = d_\rho(t)$ it is sufficient to consider the region $|t - t_\rho| < \varepsilon$, $\arg(|t - t_\rho|) > \phi$ and first suppose that $t < t_\rho$ is real. We will use a contour $\mathcal{C}(t) = \mathcal{C}_1(t) \cup \mathcal{C}_2(t) \cup \mathcal{C}_3(t)$, where $\mathcal{C}_1(t) = [\delta_\rho, s_\rho]$, $\mathcal{C}_2(t) = [s_\rho, s_\rho + e^{i\pi}(s_\rho - \delta_\rho)]$, $\mathcal{C}_3(t)$ is a circle $\{s : |s| = \delta_\rho, \arg(s) \ne 0\}$ and $\delta_\rho = \delta^{1/r}$ for some $\delta < z_\rho$ such that $c(t/s^p, s^r)$ is analytic for $|s| = \delta_\rho$ and $t < t_\rho$. Set

$$g_\rho(t) = \frac{1}{2\pi i}\int_{\mathcal{C}_3(t)} c\left(\frac{t}{s^p}, s^r\right)\frac{ds}{s}. \tag{3.3}$$

Then it is easy to see that $g_\rho(t)$ can be analytically continued in $|t - t_\rho| < \varepsilon$. Furthermore $g_\rho(t)$ can be transformed to

$$g_\rho(t) = \frac{1}{r}\sum_{j=1}^{r}\frac{1}{2\pi i}\int_{\mathcal{B}_{3,j}(t)} c\left(\frac{t}{v^\rho}, v\right)\frac{dv}{v} \tag{3.4}$$

by substituting $v = s^r$, where $\mathcal{B}_{3,j}(t) = [\mathcal{C}_{3,j}(t)]^r$ and $\mathcal{C}_{3,j}(t) = \mathcal{C}_3(t) \cap \{s : \arg(s) \in (2\pi(j-1)/r, 2\pi j/r]\}$. If we set

$$a_\rho(t) = \frac{1}{2\pi i}\int_{\mathcal{A}(t)} c\left(\frac{t}{v^\rho}, v\right)\frac{dv}{v}, \tag{3.5}$$

where $\mathcal{A}(t) = [\delta, z_\rho] \cup [z_\rho, z_\rho + e^{i\pi}(z_\rho - \delta)]$, we have

$$d_\rho(t) = \frac{1}{r}\,a_\rho(t) + g_\rho(t) \tag{3.6}$$

for $\rho = p/r$, $\gcd(p, r) = 1$. Now it is possible to prove

Lemma 2. *$a_\rho(t)$ has radius of convergence t_ρ and the following local behaviour:*

$$\begin{aligned} a_\rho(t) &= \overline{a}_\rho(t) + \frac{-1}{2\pi^2}\frac{g(z_\rho)}{\sigma(z_\rho)}\left(1-\frac{t}{t_\rho}\right)\log\left(1-\frac{t}{t_\rho}\right) \\ &\quad + O\left((1-t/t_\rho)^2\log(1-t/t_\rho)\right), \end{aligned} \tag{3.7}$$

where $\overline{a}_\rho(t)$ is analytic for $|t-t_\rho|<\varepsilon$ and $g(z)$ and $\sigma(z)$ are defined in (2.13) and (2.11). The O-constant is uniform in some neighbourhood $U(\rho)$ of ρ.

Proof. The singularities of $c(t/v^\rho, v)$ ($t<t_\rho$ fixed) are the solutions of

$$\begin{aligned} c &= G(c, t/v^\rho, v) \\ 1 &= G_c(c, t/v^\rho, v) \end{aligned} \tag{3.8}$$

resp. of $f_2(v) = t/v^\rho$. But $f_2'(z_\rho) = -\rho t_\rho/z_\rho^{\rho+1}$, that is of course equivalent to $z_\rho G = \rho x_\rho G_x$, and (2.10) imply that there are locally two singularities with expansions

$$\begin{aligned} v_1(t) &= z_\rho - v_0\sqrt{t_\rho - t}\,(1+(t_\rho-t)w_1(t)) + (t_\rho-t)w_2(t), \\ v_2(t) &= z_\rho + v_0\sqrt{t_\rho - t}\,(1+(t_\rho-t)w_1(t)) + (t_\rho-t)w_2(t), \end{aligned} \tag{3.9}$$

where

$$v_0 = \left(\frac{2}{\rho(1+\rho)x_\rho z_\rho^{\rho-2} - f_2''(z_\rho)z_\rho^\rho}\right)^{1/2}. \tag{3.10}$$

By (2.23)

$$c\left(\frac{t}{v^\rho}, v\right) = f_1(v) - \left(\left[\frac{2G_x}{G_{cc}}\right](f_1(v), f_2(v), v)\right)^{1/2}\sqrt{f_2(v)-\frac{t}{v^\rho}} + \cdots, \tag{3.11}$$

where

$$\begin{aligned} f_2(v) - t/v^\rho &= h(v)(v-v_1(t))(v_2(t)-v) \\ &= h(v)\Big(v_0^2(t_\rho-t)(1+(t_\rho-t)w_1(t)^2)^2 \\ &\qquad\qquad - (v-(z_\rho+(t_\rho-t)w_2(t))^2\Big) \\ &= h(v)\left(\overline{v}(t) - (v-\overline{\overline{v}}(t))^2\right) \end{aligned} \tag{3.12}$$

and $h(t)$ is an analytic function with $h(z_\rho) = (\rho(1+\rho)x_\rho z_\rho^{-2} - f_2''(z_\rho))/2$. So $a_\rho(t)$ can be approximated by

$$\frac{2i}{2\pi i}\sqrt{\frac{2G_x}{G_{cc}}}\frac{\sqrt{h(z_\rho)}}{z_\rho}\int_\delta^{v_1(t)}\sqrt{(v-\overline{\overline{v}}(t))^2-\overline{v}(t)}\,dv. \tag{3.13}$$

The non-analytic part of the integral in (3.13) can be calculated explicitely and is given by

$$-\frac{v_0^2}{4}(t_\rho-t)\log(t_\rho-t) + O\left((t_\rho-t)^2\log(t_\rho-t)\right). \tag{3.14}$$

This gives (3.7) for $t < t_\rho$. A more detailed analysis shows that the non-analytic part has an expansion of the form

$$\sum_{m=1}^{\infty} v_{\rho,i}(t_\rho - t)^m \log(t_\rho - t), \tag{3.15}$$

where the coefficients $v_{\rho,i}$ depend continuously on ρ. Since both functions are analytic in $|t - t_\rho| < \varepsilon$, $|\arg(t - t_\rho)| < \phi$, (3.15) is the expansion for this region, too. So we are done.

So $t = t_\rho e^{2\pi i j/r}$ $(j = 1, 2, \ldots, r)$ are the only singularities of $d_\rho(t)$ on the circle of convergence. Thus we can apply a transfer lemma (see [FO]) to get

$$c_{n,\rho n} = \frac{1}{2\pi n^2} \frac{g(z_\rho)}{\sigma(z_\rho)} (x_\rho z_\rho^\rho)^{-n} \left(1 + O\left(n^{-1}\right)\right) \tag{3.16}$$

uniformly for $\rho \in [\alpha, \beta]$. That is of course the same result as (2.12), even with a better error term. If $\mu(1) \in (\alpha, \beta)$ it is easy to show that (3.16) implies asymptotic normality.

Remark 6. Kirschenhofer's method is not so easy to handle as Bender's method but it should be noticed that Kirschenhofer's method gives a better error term and that it also works if there is no asymptotic normality. For example, in [K3] $\sigma_n^2 \sim c n^2$. In this case it seems to be impossible to find asymptotic distributions by considering $\varphi_n(z)$. These are two reasons why this method has been included in this paper.

4. Independent and maximal independent subsets of trees

4.1. Independent subsets. As proposed in the introduction the generating function $c(x, z)$ of the total number c_{nk} of independent subsets of size k of trees of size n in a given simply generated family of trees satisfies a functional equation

$$c = xz\varphi(x\varphi(c)) + x\varphi(c) = G(c, x, z), \tag{4.1}$$

where $\varphi(t) = 1 + \varphi_1 t + \cdots$ with $\varphi_i \geq 0$ characterizes the family of trees. Note that $d = \gcd\{m > 0 : \varphi_m > 0\}$ and $l = 1$. Suppose that the radius of convergence of $\varphi(t)$ is large enough that $G(c, x, z)$ is regular at the positive solution of (2.9) if z varies in a neighbourhood of $z_0 = 1$. Then all assumptions of Theorem 3 are satisfied and we can conclude that the distribution of independent subsets of size k of trees of size n is asymptotically normal. Set $\tau = f_1(1)$ and $q = f_2(1)$. Then μ_n and σ_n^2 can be evaluated asymptotically by

$$\begin{aligned} \mu_n &= \frac{\varphi(q\varphi(\tau))}{\varphi(q\varphi(\tau)) + q\varphi'(q\varphi(\tau))\varphi(\tau) + \varphi(\tau)} n + O(1) \\ \sigma_n^2 &= \sigma^2 n + O(1) \end{aligned} \tag{4.2}$$

for $n \equiv 1 \mod d$, where σ^2 is given by (2.11). Furthermore there is a bivariate asymptotic expansion for c_{nk}.

Now let $\varphi(t) = 1/(1-t)$. Then (2.18) has solution

$$\begin{aligned} c_\rho &= \frac{1+\rho^2}{2} \\ x_\rho &= \frac{(1-\rho)^2(1+\rho)}{4} \\ z_\rho &= \frac{\rho(1+\rho)}{(1-\rho)^2}. \end{aligned} \tag{4.3}$$

Thus

$$g(h(\rho)) = \frac{(1+\rho)^2}{2}\left(\frac{1-\rho}{2(3\rho+1)}\right)^{1/2} \tag{4.4}$$

and

$$\sigma(h(\rho)) = \left(\frac{\rho(1-\rho)(1+\rho)}{3\rho+1}\right)^{1/2}. \tag{4.5}$$

So we have uniformly for $k/n \in [\varepsilon, 1-\varepsilon]$ ($\varepsilon > 0$ arbitrary)

$$\begin{aligned} c_{nk} &= \frac{1}{4\sqrt{2}\pi}\frac{1}{n^2}\frac{\left(1+\frac{k}{n}\right)^{3/2}}{\left(\frac{k}{n}\right)^{1/2}}\left[\frac{4}{\left(1-\frac{k}{n}\right)^2\left(1+\frac{k}{n}\right)}\right]^n\left[\frac{\left(1-\frac{k}{n}\right)^2}{\frac{k}{n}\left(1+\frac{k}{n}\right)}\right]^k \cdot \\ &\qquad \cdot\left(1+O\left(n^{-1}\right)\right) \\ &= \frac{1}{4\sqrt{2}\pi}\frac{n^{3(n-1)}4^n}{k^{k+1/2}(n-k)^{2(n-k)}(n+k)^{n+k-3/2}}\left(1+O\left(n^{-1/2}\right)\right) \end{aligned} \tag{4.6}$$

that is of course the same asymptotic formula that can be obtained by using (1.2) and Stirling's formula. Since there are $\frac{1}{n}\binom{2n-2}{n-1}$ planted plane trees of size n the average number of independent subsets of size k in trees of size n is approximately

$$\frac{1}{\sqrt{2\pi}}\frac{n^{3(n-1/2)}}{k^{k+1/2}(n-k)^{2(n-k)}(n+k)^{n+k-3/2}}. \tag{4.7}$$

4.2. Maximal independent subsets. A subset I of a graph G is called maximal independent if I is independent and every subset $H \neq I$ with $I \subseteq H$ is not independent. In [MM1] it is shown that the functional equation for the generating function $c(x,z)$ of the total number of maximal independent subsets reads as

$$\begin{aligned} c &= xz\varphi(x\varphi(c)) + x\varphi(c) - x\varphi(c - xz\varphi(x\varphi(c))) \\ &= G(c,x,z). \end{aligned} \tag{4.8}$$

Notice that the coefficients of $G(c,x,z)$ need not be non-negative. But the generating function $d(x,z)$ that corresponds to those maximal independent subsets that do not contain the root satisfies

$$\begin{aligned} d &= x\varphi(d + xz\varphi(d + x\varphi(d))) - x\varphi(d) \\ &= H(d,x,z) \end{aligned} \tag{4.9}$$

and $c(x,z)$ can be evaluated by

$$\begin{aligned} c &= d + xz\varphi(d + x\varphi(d)) \\ &= F(d,x,z). \end{aligned} \tag{4.10}$$

Since the coefficients of the expansion of $H(d,x,z)$ are non-negative (see [MM1]) we can apply Theorem 3 if the radius of convergence of $\varphi(t)$ is large enough. Again $d = \gcd\{m > 0 : \varphi_m > 0\}$ and $l = 1$.

Now let $\varphi(t) = 1/(1-t)$. First we derive an explicit formula by using Lagrange's inversion formula. (4.9) can be transformed to

$$z = \frac{d}{x\left(\frac{1}{(1-d)^2(1-x(1-d)^{-2}))} - \frac{1}{1-d}\right)} = \frac{d}{x\,u(d,x)}. \tag{4.11}$$

Furthermore by (4.10)

$$\begin{aligned} F_d(d,x,z) &= 1 + z\left(\frac{-x}{(1-d)^2\left(1-\frac{x}{(1-d)^2}\right)} + \frac{2dx}{(1-d)^2\left(1-\frac{x}{(1-d)^2}\right)^2}\right) \\ &= 1 + z\,v(d,x). \end{aligned} \tag{4.12}$$

So we have

$$\begin{aligned} c_{nk} &= \frac{1}{k}[x^n y^{k-1}]x^k u(y,x)^k \\ &\quad + \frac{1}{k-1}[x^n y^{k-2}]x^{k-1} v(y,x) u(y,x)^{k-1}, \end{aligned} \tag{4.13}$$

where $[x^n y^m]f(x,y)$ denotes the coefficient f_{nm} of the expansion of $f(x,y) = \sum f_{ij} x^i y^j$. After some calculations we get

$$\begin{aligned} c_{nk} &= \frac{1}{k}\sum_{l=0}^{k}(-1)^{k-l}\binom{k}{l}\binom{n+l-k-1}{n-k}\binom{2n+l-2}{k-1} \\ &\quad - \frac{1}{k-1}\sum_{l=0}^{k-1}(-1)^{k-l-1}\binom{k-1}{l}\binom{n+l-k}{n-k}\binom{2n+l-2}{k-2} \\ &\quad + \frac{2}{k-1}\sum_{l=0}^{k-1}(-1)^{k-l-1}\binom{k-1}{l}\binom{n+l-k+1}{n-k}\binom{2n+l-3}{k-3} \end{aligned} \tag{4.14}$$

The first sum corresponds to those maximal independent subsets that do not contain the root. At a first glance it seems to be hopeless to get bivariate asymptotic expansions of these alternating sums directly since there is no dominating term in general. Only if $k = o(n^{2/3})$ it is easy to see that the last term in each sum is dominating. So we have to use Theorem 3. System (2.16) has the following solution:

$$\begin{aligned} c_\rho &= \frac{(2+\rho(1-\rho))W - (1+\rho)(4-12\rho+3\rho^2-\rho^3)}{16\rho} \\ x_\rho &= \frac{12-48\rho+43\rho^2-19\rho^3+5\rho^4-\rho^5+(2-\rho)(5-2\rho+\rho^2)W}{32(1-\rho)} \\ z_\rho &= \frac{2-7\rho(1-\rho)-(1-2\rho)W}{2\rho(1-\rho)^2}, \end{aligned} \tag{4.15}$$

where $W = \sqrt{4 - 12\rho(1-\rho) + \rho^2(1-\rho)^2}$. Thus

$$g(h(\rho)) = \left(\frac{p_1(\rho) - p_2(\rho)W}{256(4 - 9\rho + 15\rho^2 - 12\rho^3 + 6\rho^4)} \right)^{1/2}, \tag{4.16}$$

where $p_1(\rho) = 64 + 240\rho - 784\rho^2 + 1432\rho^3 - 1632\rho^4 + 1275\rho^5 - 719\rho^6 + 270\rho^7 - 90\rho^8 + 15\rho^9 - 3\rho^{10}$ and $p_2(\rho) = 32 - 88\rho + 228\rho^2 - 322\rho^3 + 269\rho^4 - 138\rho^5 + 60\rho^6 - 12\rho^7 + 3\rho^8$, and

$$\sigma(h(\rho)) = \left(\frac{\rho(1-\rho)W(6 - 7\rho(1-\rho) - W)}{4(4 - 9\rho + 15\rho^2 - 12\rho^3 + 6\rho^4)} \right)^{1/2}. \tag{4.17}$$

So $\mu(1) = 1/2$ and $\sigma(1)^2 = (\sqrt{17} - 1)/2^5$ and it is possible to find an explicit asymptotic expansion for (4.14) uniformly for $k/n \in [\varepsilon, 1-\varepsilon]$. For example we have

$$c_{n,n/2} \sim \frac{1}{2\pi n^2} \left(\frac{7 \cdot 1657\sqrt{17} + 17 \cdot 137}{2^{11}17} \right)^{1/2} \left(\frac{51\sqrt{17} + 107}{2^6} \right)^n. \tag{4.18}$$

5. A multivariate Darboux method

The crucial point in the proof of Theorem 3 was to establish an expansion of type (2.1). This has been done by using the expansion (2.23) and Darboux's theorem. This may be called a multivariate Darboux-method. We will formulate this principle for multivariate generating functions

$$c(x, z) = \sum_{n,k} c_{nk} x^n z^k, \tag{5.1}$$

where $z = (z_1, \dots, z_m)$, $k = (k_1, \dots, k_m)$, and $z^k = z_1^{k_1} \cdots z_m^{k_m}$. (Similarly e^z and $|z|$ should be interpreted as $(e^{z_1}, \dots, e^{z_m})$ and $(|z_1|, \dots, |z_m|)$.)

As in [FO] say that a function $L(u)$ is of slow variation at infinity if it satisfies following conditions:

V1. There exists a positive real number u_0 and an angle ϕ with $0 < \phi < \pi/2$ such that $L(u)$ is $\neq 0$ and analytic in the domain $\{u : |\arg(\phi)| \le \pi - \phi\}$.

V2. There exists a function $\varepsilon(u)$, defined for $x \ge 0$ with $\lim_{u\to\infty} \varepsilon(u) = 0$, such that for all $\vartheta \in [\phi - \pi, \pi - \phi]$ and $u \ge u_0$, we have

$$\left| \frac{L(ue^{i\vartheta})}{L(u)} - 1 \right| < \varepsilon(u) \quad \text{and} \quad \left| \frac{L(u \log^2 u)}{L(u)} - 1 \right| < \varepsilon(u). \tag{5.2}$$

Theorem 4. *Let $c(x, z)$ be the generating function for c_{nk} and suppose that $c(x, z)$ has positive radius of convergence $r(z)$ for $z = (z_1, \dots, z_m) \in [a, b] = [a_1, b_1] \times \cdots \times [a_m, b_m]$ $(0 < a_i < b_i)$, that there is only one singularity $x = f(z)$ on the circle of convergence $|x| = r(z)$, and that $c(x, z)$ has an expansion of the following form:*

$$c(x, z) = u(x, z) + g(z) A\left(\frac{1}{1 - x/f(z)} \right) + o\left(A\left(\frac{1}{1 - x/f(z)} \right) \right) \tag{5.3}$$

for $x/f(z) \to 1$, $z \in R(a, b, \phi) = \{z = (z_1, \dots, z_m) : |z| \in [a, b], |arg(z_i)| < \phi\}$ and $x \in T(f(z), \varepsilon, \phi) = \{x : |f(z) - x| < \varepsilon, |arg(x - f(z))| < \phi\}$ for some $\varepsilon, \phi > 0$, *where* $A(u) = u^r L(u)$, $r \neq -1, -2, \ldots$, $L(u)$ *is of slow variation, and* $u(x, z)$, $f(z)$, *and* $g(z) \neq 0$ *are analytic for* $z \in R(a, b, \phi)$ *and* $|f(z) - x| < \varepsilon$. *Set*

$$\mu(z) = -\nabla \log f(e^s)|_{e^s = z}, \tag{5.4}$$

suppose that the matrix

$$\Sigma(z) = \left(-\frac{\partial^2}{\partial s_i \partial s_j} \log f(e^s)|_{e^s = z} \right)_{i,j=1}^{m} \tag{5.5}$$

is regular for $z \in R(a, b, \phi)$, *and that there exists a* $\delta > 0$ *such that* $c(x, z)$ *is analytic and bounded for* $|z| \in [a, b]$, $z \notin R(a, b, \phi)$, $|x| \leq r(z)(1 + \delta)$. *Then* $\det \Sigma(z) > 0$ *and we have*

$$c_{nk} \sim \frac{g\left(h\left(\frac{k}{n}\right)\right)}{\sqrt{(2\pi n)^m \det \Sigma\left(h\left(\frac{k}{n}\right)\right)}} \, \frac{A(n)}{\Gamma(r) n} \, \frac{1}{f\left(h\left(\frac{k}{n}\right)\right)^n h\left(\frac{k}{n}\right)^k} \tag{5.6}$$

uniformly for $k/n \in [\mu(a), \mu(b)]$, *where* $h(t)$ *is the inverse function of* $\mu(z)$.

Sketch of the Proof. By [FO, Theorem 5] we have

$$\varphi_n(z) \sim \frac{A(n)}{\Gamma(r) n} \, g(z) \, f(z)^{-n}. \tag{5.7}$$

So we can use [BR, Theorem 2] combined with the proof of [B, Theorem 3].

Remark 7. For example, functions like $L(u) = \log^\delta u \log \log^\theta u$ are of slow variation. In these cases it is easy to get an error term of explicit order of magnitude. If

$$c(x, z) = u(x, z) + g(z) A\left(\frac{1}{1 - x/f(z)} \right) + O\left(B\left(\frac{1}{1 - x/f(z)} \right) \right), \tag{5.8}$$

where $A(u) = u^r \log^\delta u \log\log^\theta u$, $B(u) = u^R \log^\Delta u \log\log^\Theta u$, and $r, R \neq -1, -2, \ldots$, then c_{nk} equals (5.6) times the error term

$$\left(1 + O\left(n^{-1/2} \right) + O\left(\frac{B(n)}{A(n)} \right) \right). \tag{5.9}$$

References

[B] Bender, E.A., *Central and Local Limit Theorems Applied to Asymptotic Enumeration*, J. Comb. Th. (A) **15** (1973), 91–111.

[BR] Bender, E.A., and L.B. Richmond, *Central and Local Limit Theorems Applied to Asymptotic Enumeration II: Multivariate Generating Functions*, J. Comb. Th. (A) **34** (1983), 255–265.

[Dr] Drmota, M., *On Generalized Fibonacci Numbers of Trees*, in: Applications of Fibonacci Numbers Vol. 3, Kluwer Academic Press (1990), 63–76.

[FO] Flajolet, Ph., and A. Odlyzko, *Singularity Anlalysis of Generating Functions*, SIAM J. Disc. Math. **3** (1990), 216–240.

[K1] Kirschenhofer, P., *On the Height of Leaves in Binary Trees*, J. Comb. Inf. Syst. Sci. **8** (1983), 44–60.

[K2] Kirschenhofer, P., *On the Average Shape of Simply Generated Families of Trees*, J. Graph Th. **7** (1983), 311–323.

[K3] Kirschenhofer, P., *A Tree Enumeration Problem Involving the Asymptotics of the "Diagonals" of a Power Series*, Ann. Discr. Math. **33** (1987), 157–170.

[KPT] Kirschenhofer, P., H. Prodinger, and R.F. Tichy, *Fibonacci Numbers of Graphs III: Planted Plane Trees*, in: Fibonacci Numbers and Their Applications, Reidel, Dortrecht— Boston (1986), 105–120.

[MM1] Meir, A., and J.W. Moon, *On Maximal Independent Sets of Nodes in Trees*, J. Graph Th. **12** (1988), 265–283.

[MM2] Meir, A., and J.W. Moon, *On an Asymptotic Method in Enumeration*, J. Comb. Th. **51** (1989), 77–89.

Michael Drmota
Department of Discrete Mathematics
Technichal University of Vienna
Wiedner Hauptstrasse 8–10/118
A-1040 Vienna, AUSTRIA
E-mail: mdrmota@email.tuwien.ac.at