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THE APPLICATION OF LAGRANGIAN METHODS TO THE ENUMERATION OF LABELLED TREES WITH RESPECT TO EDGE PARTITION

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1. Introduction. In an earlier paper [6] we considered the application of Lagrangian methods to the enumeration of plane rooted trees with given colour partition. We obtained an expression which generalised Tutte's result [9], and a correspondence, which, when specialised, gives the de Bruijn–van Aardenne Ehrenfest–Smith–Tutte Theorem [1]. A corollary of these results is a one-to-one correspondence [4], between trees and generalised derangements, for which no combinatorial description has yet been found.

In this paper we extend these methods to the enumeration of rooted labelled trees to demonstrate how another pair of well-known and apparently unrelated theorems may be obtained as the result of a single enumerative approach. In particular, we show that a generalisation of Good's result [3], also considered by Knuth [7], and the matrix tree theorem [8] have a common origin in a single system of functional equations, and that they correspond to different coefficients in the power series solution. We observe that this system of functional equations is a multivariate generalisation of the familiar functional equation $T(x) = x \exp T(x)$, associated with Cayley's result for labelled rooted trees.

By considering the enumeration of paths in a graph we may also derive the numbers of Eulerian and Hamiltonian circuits of a graph. Again, these results correspond to different terms in the power series solution of a single functional equation. The details are oblique to the present paper, and are given elsewhere [5].

We use a familiar decomposition of rooted trees to obtain a system of functional equations. This system is solved by means of the Lagrange Theorem (Theorem 2.2) and a specialisation (Corollary 2.3) which appears to be of considerable utility in this connexion.

A K-coloured rooted tree is said to have *edge-partition* $\mathbf{D}$ if $\mathbf{D}$ is a $K \times K$ matrix whose (i, j)-element, d_{ij}, is the number of edges directed away from the root, from a vertex of colour i to a vertex of colour j. Throughout this paper, the number of vertices of colour i in a tree with

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root colour c is

$$n_i = \sum_{j=1}^{K} d_{ji} + \delta_{ic}$$

and $N = n_1 + \ldots + n_K$, the number of vertices in the tree. Let $\mathbf{n} = (n_1, \ldots, n_K)$, and $\mathbf{q} = (q_1, \ldots, q_K)$ where $q_i = \sum_{j=1}^{K} d_{ij}$ for $1 \leqq i \leqq K$.

The following notational conventions are used. If $\mathbf{A}$ is a $K \times K$ matrix with elements a_{ij}, we write $\mathbf{A} = [a_{ij}]_{K\times K}$ and $a_{ij} = [\mathbf{A}]_{ij}$. The determinant of $\mathbf{A}$ is denoted by $|\mathbf{A}|$ or $\|a_{ij}\|$, and the (s, t)-cofactor of $\mathbf{A}$ by $\operatorname{cof}_{s,t}\mathbf{A}$. If $\mathbf{M} = [m_{ij}]_{K\times K}$ is a non-negative integer matrix then

$$\mathbf{A}^{\mathbf{M}} = \prod a_{ij}{}^{m_{ij}} \text{ and } \mathbf{M}! = \prod m_{ij}!$$

where the products are over i and j such that $1 \leqq i, j \leqq K$. If $f(\mathbf{A})$ is a power series in the elements of $\mathbf{A}$, then $[\mathbf{A}^{\mathbf{M}}]f(\mathbf{A})$ denotes the coefficient of $\mathbf{A}^{\mathbf{M}}$ in $f(\mathbf{A})$. Let $\mathbf{1}$ denote the unit vector with K components, and $[\mathbf{x}]$ denote $[\mathbf{x}^{\mathbf{1}}]$ where $\mathbf{x} = (x_1, \ldots, x_K)$.

2. The system of functional equations. We now set up the system of functional equations which will be used throughout this paper.

Let $\theta_c^{(K)}(\mathbf{D})$ denote the number of K-coloured labelled trees rooted at a vertex of colour c, and having edge-partition $\mathbf{D}$. We obtain a system of functional equations for $\theta_c^{(K)}(\mathbf{D})$ by using a familiar decomposition of rooted labelled trees.

LEMMA 2.1.

$$\theta_c^{(K)}(\mathbf{D}) = \left[\mathbf{A}^{\mathbf{D}}\mathbf{x}^{\mathbf{n}}\frac{z^N}{N!}\right]f_c(\mathbf{A}, \mathbf{x}, z)$$

where $f_1, \ldots, f_K$ *satisfy*

$$f_i = zx_i \exp\left\{\sum_{j=1}^{K} a_{ij}f_j\right\} \quad \textit{for } i = 1, \ldots, K.$$

Proof. Consider a K-coloured rooted labelled tree, t, with root degree k and root colour i. The tree t consists of a set $\{t_1, \ldots, t_k\}$ of k K-coloured rooted labelled trees whose roots are joined to a vertex of colour i. Let $a_{p,q}$ be an indeterminate marking an edge from a vertex of colour p to a vertex of colour q. Let x_i mark a vertex of colour i, and z mark any vertex. These trees are enumerated by $zx_i(a_{i1}f_1 + \ldots + a_{iK}f_K)^k/k!$ since each of the different orderings of $t_1, \ldots, t_k$, of which these are $k!$, since the trees are labelled, corresponds to t. The result follows.

The following two results are used in the solution of this system of functional equations. The first is the multivariate extension of the Lagrange theorem, and the second is a specialisation to the monomial case.

THEOREM 2.2. ([**2**], [**10**]). *Let* $\boldsymbol{\phi} = (\phi_1, \ldots, \phi_\kappa)$ and γ *be formal power series in the indeterminates* $\boldsymbol{\xi} = (\xi_1, \ldots, \xi_\kappa)$ *and with no terms with negative exponents. Suppose that* $\boldsymbol{\zeta} = (\zeta_1, \ldots, \zeta_\kappa)$ *satisfies* $\xi_i = \zeta_i\phi_i(\boldsymbol{\xi})$ *for* $i = 1, \ldots, \kappa$. *Then where* $\nu = (\nu_1, \ldots, \nu_\kappa)$,

$$[\boldsymbol{\zeta}^{\boldsymbol{\nu}}]\gamma(\boldsymbol{\xi}(\boldsymbol{\zeta})) = [\boldsymbol{\xi}^{\boldsymbol{\nu}}]\gamma(\boldsymbol{\xi})\boldsymbol{\phi}^{\boldsymbol{\nu}}(\boldsymbol{\xi}) \left\| \delta_{ij} - \frac{\xi_j}{\phi_i(\boldsymbol{\xi})} \frac{\partial \phi_i(\boldsymbol{\xi})}{\partial \xi_j} \right\|.$$

The next corollary is useful in allowing us to avoid the extraction of coefficients from the determinant in Theorem 2.2.

COROLLARY 2.3. ([**6**]). *Under the conditions of Theorem* 2.2 *further suppose that* $\phi_i(\boldsymbol{\xi})$ *is independent of* ξ_j *for each* $(i, j) \in \mathscr{S} \subseteq \{1, \ldots, \kappa\}^2$. *Then*

$$[\boldsymbol{\zeta}^{\boldsymbol{\nu}}]\boldsymbol{\xi}^{\mathbf{r}} = (\nu_1 \ldots \nu_\kappa)^{-1} \sum_{\boldsymbol{\mu}} \|\delta_{ij}\nu_i - \mu_{ij}\| \prod_{i=1}^{\kappa} ([\xi_1^{\mu_{i1}} \ldots \xi_\kappa^{\mu_{i\kappa}}]\phi_i^{\nu_i})$$

where the summation is over all non-negative integer $\kappa \times \kappa$ *matrices such that*

$$\sum_{i=1}^{\kappa} \mu_{ij} = \nu_j - r_j, j = 1, \ldots, \kappa \quad \textit{and} \quad \mu_{ij} = 0 \textit{ for each } (i, j) \in \mathscr{S}.$$

3. ***K*-coloured trees with given edge partition.** The number $\theta_c^{(K)}(\mathbf{D})$ may be given explicitly. The result is given in Theorem 3.1, and a specialisation in Corollary 3.2.

THEOREM 3.1.

$$\theta_c^{(K)}(\mathbf{D}) = N!\,\mathbf{n}^{\mathbf{q}-\mathbf{1}}\,(\mathbf{D}!)^{-1}\,\mathrm{cof}_{cc}[\delta_{ij}n_i - d_{ij}]_{K\times K}.$$

Proof. From Lemma 2.1 and Corollary 2.3 we obtain

$$\theta_c^{(K)}(\mathbf{D}) = N!(n_1 \ldots n_K)^{-1} \sum \|\delta_{ij}n_i - \mu_{ij}\|$$
$$\times \prod_{i=1}^{K} \left\{ [a_{i1}^{d_{i1}} \ldots a_{iK}^{d_{iK}}][f_1^{\mu_{i1}} \ldots f_K^{\mu_{iK}}] \exp\left(n_i \sum_{j=1}^{K} a_{ij} f_j\right) \right\}$$

where

$$\sum_{i=1}^{K} \mu_{ij} = n_j - \delta_{jc},$$

and the result follows.

Next we consider labelled abstract K-coloured trees rooted at a vertex of colour c, with n_i non-root vertices of colour i and in which there are arbitrary restrictions on colour adjacencies. The number of such trees is denoted by $\lambda_c^{(K)}(\mathbf{n}, \mathbf{T})$, where $[\mathbf{T}]_{ij} = T_{ij} = 1$ if edges directed from a vertex of colour i to a vertex of colour j are allowed and $T_{ij} = 0$ otherwise. In the next corollary we obtain $\lambda_c^{(K)}(\mathbf{n}, \mathbf{T})$, a result given by

Good [**3**]. Knuth [**7**] later gave a combinatorial proof of the result by means of Prüfer codes. We obtain the result by summing $\theta_c^{(K)}(\mathbf{D})$ over $\mathbf{D}$.

COROLLARY 3.2.

$$\lambda_c^{(K)}(\mathbf{n}, \mathbf{T}) = N!(\mathbf{n}!)^{-1} \operatorname{cof}_{cc}\left[\delta_{ij}\left(\sum_{l=1}^{K} n_l T_{lj}\right) - n_i T_{ij}\right]_{K\times K} \times \prod_{j=1}^{K}\left(\sum_{i=1}^{K} n_i T_{ij}\right)^{n_j-1}$$

Proof. The required number is clearly, from Theorem 3.1,

$$\lambda_c^{(K)}(\mathbf{n}, \mathbf{T}) = \sum_{\mathbf{D}} \theta_c^{(K)}(\mathbf{D})$$

where the sum is over all $\mathbf{D}$ such that

$$\sum_{i=1}^{K} d_{ij} = n_j - \delta_{jc} \quad \text{and} \quad d_{ij} = 0 \text{ when } T_{ij} = 0.$$

Thus, if $\boldsymbol{\delta}_c = (\delta_{c1}, \ldots, \delta_{cK})$,

$$\begin{aligned}\lambda_c^{(K)}(\mathbf{n}, \mathbf{T}) &= N!(n_1 \ldots n_K)^{-1}[\mathbf{x}^{\mathbf{n}-\boldsymbol{\delta}_c}] \sum_{\mathbf{D}\geq \mathbf{0}} \left\{\prod_{i=1}^{K}\prod_{j=1}^{K} (n_i x_j T_{ij})^{d_{ij}} (d_{ij}!)^{-1}\right\} \\ &\quad \times \operatorname{cof}_{cc}\left[\delta_{ij}\left(\sum_{l=1}^{K} d_{lj} T_{lj}\right) - d_{ij} T_{ij}\right]_{K\times K} \\ &= N!(n_1 \ldots n_K)^{-1}[\mathbf{x}^{\mathbf{n}-\boldsymbol{\delta}_c}] \exp\left\{\sum_{i=1}^{K}\sum_{j=1}^{K} n_i x_j T_{ij}\right\} \\ &\quad \times \operatorname{cof}_{cc}\left[\delta_{ij}\left(\sum_{l=1}^{K} n_l x_j T_{lj}\right) - n_i x_j T_{ij}\right]_{K\times K}\end{aligned}$$

since

$$\sum_{\mathbf{i}\geq \mathbf{0}} \mathbf{x}^{\mathbf{i}}(\mathbf{i}!)^{-1} g(\mathbf{i}) = g(\mathbf{x}) \exp\left(\sum_j x_j\right),$$

where $g(\mathbf{x})$ is multilinear. Accordingly we have

$$\lambda_c^{(K)}(\mathbf{n}, \mathbf{T}) = N!(n_1 \ldots n_K)^{-1} \operatorname{cof}_{cc}\left[\delta_{ij}\left(\sum_{l=1}^{K} n_l T_{lj}\right) - n_i T_{ij}\right]_{K\times K} \times [\mathbf{x}^{\mathbf{n}-\mathbf{1}}] \exp\left\{\sum_{j=1}^{K} x_j \sum_{i=1}^{K} n_i T_{ij}\right\}$$

and the result follows.

4. The matrix tree theorem. We now obtain an enumerative proof of the matrix tree theorem. Although a number of proofs ([**8**], [**3**], among others) are available we include this proof since it may be obtained directly from Lemma 2.1. We consider first the stronger form of the theorem in which edges are directed and may be marked with indeterminates.

THEOREM 4.1. (The matrix tree theorem.) *The number of trees rooted at c on the vertex set* $\{1, \ldots, K\}$ *with* m_{ij} *occurrences of the edge ij directed away from the root is*

$$[\mathbf{A}^{\mathbf{M}}] \operatorname{cof}_{cc}[\delta_{ij}\alpha_j - a_{ij}]_{K\times K} \quad \textit{where} \quad \alpha_j = \sum_{i=1}^{K} a_{ij}.$$

Proof. Let $f_i(\mathbf{A}, \mathbf{x}, 1) = F_i(\mathbf{A}, \mathbf{x})$, so the required number is $[\mathbf{A}^{\mathbf{M}}\mathbf{x}]F_c(\mathbf{A}, \mathbf{x})$ since $[(z^K/K!)\,\mathbf{x}]f_c = K![\mathbf{x}]F_c$ and we remove the labelling. From Lemma 2.1 and Theorem 2.2 we have

$$[\mathbf{x}]F_c = [\mathbf{F}]F_c\left\{\exp \sum_{i=1}^{K} \Phi_i\right\}\|\delta_{ij} - F_j a_{ij}\| \quad \text{where} \quad \Phi_i = \sum_{j=1}^{K} a_{ij}F_j.$$

Thus

$$\begin{aligned}
[\mathbf{x}]F_c &= [\mathbf{F}]F_c\|\delta_{ij}e^{F_j\alpha_j} - a_{ij}F_je^{F_j\alpha_j}\| \\
&= [\mathbf{F}]F_c\|\delta_{ij}(\delta_{cj} + F_j\alpha_j) - a_{ij}F_j\| \\
&= [\mathbf{F}]F_c \operatorname{cof}_{cc}[\delta_{ij}F_j\alpha_j - a_{ij}F_j]_{K\times K} \\
&= \operatorname{cof}_{cc}[\delta_{ij}\alpha_j - a_{ij}]_{K\times K}.
\end{aligned}$$

By setting $K = 1$, $a_{11} = 1$, $z = 1$ and $x_1 = x$ in Lemma 2.1, we note that the number of rooted labelled trees on n vertices is $[x^n/n!]T(x)$ where $T(x) = xe^{T(x)}$. This is, of course, well-known and yields immediately Cayley's result that there are n^{n-1} rooted labelled trees on n nonroot vertices, a fact which, at the functional equation level at least, makes a striking connexion between two classical, and apparently unconnected, results.

The last corollary gives the result when the matrix $\mathbf{A}$ of indeterminates a_{ij} marking the edge ij is replaced by the adjacency matrix of a graph. This is perhaps the more familiar form of the matrix tree theorem.

COROLLARY 4.2. *The number of out-directed spanning arborescences, rooted at c, of a directed graph on the vertex set* $\{1, \ldots, K\}$ *with adjacentcy matrix* $\mathbf{A} = [\lambda_{ij}]_{K\times K}$ *is*

$$\operatorname{cof}_{cc}\left[\delta_{ij}\left(\sum_{p=1}^{K} \lambda_{pj}\right) - \lambda_{ij}\right]_{K\times K}.$$

$\left(\textit{For the in-directed case the number is } \operatorname{cof}_{cc}\left[\delta_{ij}\left(\sum_{q=1}^{K} \lambda_{iq}\right) - \lambda_{ij}\right]_{K\times K}.\right)$

Proof. This follows straightforwardly from Theorem 4.1.

For undirected graphs, for which $\mathbf{A}$ is symmetric, the result follows immediately.

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