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SEQUENCE ENUMERATION AND THE DE BRUIJN-VAN AARDENNE EHRENFEST-SMITH-TUTTE THEOREM

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1. Introduction and notation. The de Bruijn—van Aardenne Ehrenfest—Smith—Tutte theorem [**1**] is a theorem which connects the number of Eulerian dicircuits in a directed graph with the number of rooted spanning arborescences. In this paper we obtain a proof of this theorem by considering sequences over a finite alphabet, and we show that the theorem emerges from the generating function for a certain type of sequence. The generating function for the set of sequences is obtained as the solution of a linear system of equations in Section 2. The power series expansion for the solution of this system is obtained by means of the multivariate form of the Lagrange theorem for implicit functions, and is given in Section 3, together with a restatement of the theorem as a matrix identity. Corollaries of these results are given in Section 4 and include the de Bruijn—van Aardenne Ehrenfest—Smith—Tutte theorem, and an expression for the number of directed Hamiltonian cycles of a graph. In Section 5 we consider briefly some possible extensions of the matrix identity to other sequence problems.

To abbreviate some of the multivariate expressions which arise in the subsequent development, the following notational apparatus is used.

1) $\mathbf{A} = [a_{ij}]_{n\times n}$, $\mathbf{x} = (x_1, \ldots, x_n)$, $\mathbf{X} = \text{diag}\,(x_1, \ldots, x_n)$ where $\{a_{ij} | i, j = 1, 2, \ldots, n\}$ and $\{x_1, \ldots, x_n\}$ are sets of indeterminates.

2) $\mathbf{M} = [m_{ij}]_{n\times n}$, $\mathbf{k} = (k_1, \ldots, k_n)$, $\mathbf{K} = \text{diag}\,(k_1, \ldots, k_n)$ where $\{m_{ij} | i, j = 1, 2, \ldots, n\}$ and $\{k_1, \ldots, k_n\}$ are sets of non-negative integers.

3) When convenient we adopt an implied product convention in which

$\mathbf{A}^{\mathbf{M}} = \prod_{i,j=1}^{n} a_{ij}^{m_{ij}}$ and $\mathbf{M}! = \prod_{i,j=1}^{n} m_{ij}!$.

4) $[(\ldots)]_{ij}$ denotes the (i, j)-element of the matrix $(\ldots)$. $\text{cof}_{ij}(\ldots)$ denotes the (signed) cofactor of (i, j) in the matrix $(\ldots)$. $[x^n](\ldots)$ denotes the coefficient of x^n in the power series $(\ldots)$.

2. Preliminaries. We now consider the enumeration of sequences over the set $\mathscr{N} = \{1, 2, \ldots, n\}$ in the situation where, for each sequence, information concerning the frequencies of occurrence of each i and each adjacent pair ij

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for $i, j \in \mathscr{N}$ is to be retained. The following proposition sets up the appropriate generating function for this purpose.

PROPOSITION 2.1. *Let $\mathscr{S} = \mathscr{N}^*$ be the monoid of sequences over $\mathscr{N}$ with concatenation (denoted by juxtaposition) and let $\mathscr{S}^+ = \mathscr{S} \backslash \{\epsilon\}$ where ϵ is the empty sequence. Then the generating function for $\mathscr{S}^+$ is*

$$\Phi(\mathbf{x}, \mathbf{A}) = \sum_{\sigma \in \mathscr{S}^+} W(\sigma)$$

where $W(\sigma) = \mathbf{x}^{\mathbf{k}} \mathbf{A}^{\mathbf{M}}$ in which k_i is the frequency occurrence of i in σ and m_{ij} is the frequency of occurrence of ij in σ. Furthermore, if $\sigma \in \mathscr{S}^+$ begins with p and ends with q then

$$k_j = \sum_{i=1}^{n} m_{ij} + \delta_{pj} \text{ for } j = 1, 2, \ldots, n$$
$$k_i = \sum_{j=1}^{n} m_{ij} + \delta_{iq} \text{ for } i = 1, 2, \ldots, n.$$

Proof. By construction, the number of sequences in $\mathscr{S}^+$ with k_i occurrences of i for $i = 1, 2, \ldots, n$ and m_{ij} occurrences of ij for $i, j = 1, 2, \ldots, n$ is $[\mathbf{x}^{\mathbf{k}} \mathbf{A}^{\mathbf{M}}] \Phi(\mathbf{x}, \mathbf{A})$ so $\Phi(\mathbf{x}, \mathbf{A})$ is the appropriate generating function. The second part of the proposition is immediate.

The following lemma provides a means of determining this generating function.

LEMMA 2.2. *There is a unique $\mathbf{y} = (y_1, \ldots, y_n)$ which satisfies the linear system*

$$\mathbf{y}^T = \mathbf{x}^T + \mathbf{X}\mathbf{A}\mathbf{y}^T.$$

Moreover, this $\mathbf{y}$ is such that

$$y_1 + \ldots + y_n = \Phi(\mathbf{x}, \mathbf{A}).$$

Proof. Let $\mathscr{S}_i \subset \mathscr{S}^+$ be the subset of sequences of $\mathscr{S}^+$ beginning with the symbol $i \in \mathscr{N}$. Then

(1) $\quad \mathscr{S}^+ = \bigcup_{i=1}^{n} \mathscr{S}_i.$

Now each element of $\mathscr{S}_i$ may be formed in a unique way by attaching i as a prefix to a member of $\mathscr{S}$, so

(2) $\quad \mathscr{S}_i = i\mathscr{S}.$

Let $z_i = \sum_{\sigma \in \mathscr{S}_i} W(\sigma)$ so, from (1),

$$\Phi(\mathbf{x}, \mathbf{A}) = z_1 + \ldots + z_n.$$

Moreover, from (2),

$$\mathscr{S}_i = \{i\} \cup \{i \textstyle\bigcup_{j=1}^{n} \mathscr{S}_j\} \text{ for } i = 1, 2, \ldots, n$$

so $\mathbf{z} = (z_1, \ldots, z_n)$ satisfies

$$z_i = x_i + x_i \sum_{j=1}^n a_{ij} z_j,\ i = 1, 2, \ldots, n$$

which may be written

$$\mathbf{z}^T = \mathbf{x}^T + \mathbf{XAz}^T.$$

Accordingly, $\mathbf{z}$ satisfies the given linear system. Now

$$(\mathbf{I} - \mathbf{XA})\mathbf{z}^T = \mathbf{x}^T$$

and $\mathbf{I} - \mathbf{XA}$ is non-singular since $\mathbf{A}$ and $\mathbf{X}$ are matrices of indeterminates. Thus the solution is unique and the lemma follows.

3. The main theorem. The following theorem gives an explicit power series expansion for the generating function for $\mathscr{S}^+$.

THEOREM 3.1. $\Phi(\mathbf{x}, \mathbf{A}) = y_1 + \ldots + y_n$ *where*

$$y_p = \sum_{\mathbf{M}} \mathbf{x}^{\mathbf{k}} \mathbf{A}^{\mathbf{M}} |\mathbf{K} - \mathbf{M}| (\mathbf{k} - \mathbf{1})! (\mathbf{M}!)^{-1}$$

in which the summation is over all $n \times n$ non-negative integer matrices $\mathbf{M}$ *such that*

$$k_j = \sum_{i=1}^n m_{ij} + \delta_{pj},\ j = 1, 2, \ldots, n$$

providing there exists $q \in \mathscr{N}$ such that

$$k_i = \sum_{j=1}^n m_{ij} + \delta_{iq},\ i = 1, 2, \ldots, n.$$

Proof. From Lemma 2.2, the generating function is given by

$$\Phi(\mathbf{x}, \mathbf{A}) = y_1 + \ldots + y_n$$

and the summation conditions on $\mathbf{M}$ are given by Proposition 2.1. Furthermore, from Lemma 2.2, we have

$$y_i = x_i f_i(\mathbf{y}),\ i = 1, 2, \ldots, n$$

where

$$f_i(\mathbf{y}) = 1 + \sum_{j=1}^n a_{ij} y_j,\ i = 1, 2, \ldots, n.$$

Accordingly our task is to expand y_p as a function of $x_1, \ldots, x_n$ where $\mathbf{y}$ is given intrinsically in terms of $\mathbf{x}$ by the above functional equations. We use the multivariate form of the Lagrange theorem for implicit functions [**5**], which holds [**14**] for the algebra of formal power series. Let $\mathbf{f} = (f_1, \ldots, f_n)$. Then

$$\begin{aligned}[\mathbf{x}^{\mathbf{k}}] y_p &= [\mathbf{y}^{\mathbf{k}}] y_p \mathbf{f}^{\mathbf{k}} \| \delta_{ij} - (y_j/f_i)\ \partial f_i/\partial y_j \| \\ &= [\mathbf{y}^{\mathbf{k}}] y_p \| \delta_{ij} f_i^{k_i} - (y_j/k_i)\ \partial f_i^{k_i}/\partial y_j \| \\ &= \sum_{\mathbf{M}} \prod_{i=1}^n \{[y_1^{m_{i1}} \ldots y_n^{m_{in}}] f_i^{k_i}\} \| \delta_{ij} - m_{ij}/k_i \|\end{aligned}$$

where the summation is taken over $\mathbf{M}$ such that

$$\sum_{i=1}^{n} m_{ij} = k_j - \delta_{jp}, \text{ for } j = 1, 2, \ldots, n.$$

Clearly

$$\sum_{j=1}^{n} m_{ij} \leqq k_i, \text{ for } i = 1, 2, \ldots, n$$

but since $\sum_{i=1}^{n} \sum_{j=1}^{n} m_{ij} = \sum_{j=1}^{n} k_j - 1$, then

$$\sum_{j=1}^{n} m_{ij} = k_i - \delta_{iq} \text{ for some } q \in \{1, 2, \ldots, n\}.$$

Thus

$$[\mathbf{A}^{\mathbf{M}}\mathbf{x}^{\mathbf{k}}]y_p = |\mathbf{K} - \mathbf{M}| \prod_{l=1}^{n} \frac{1}{k_l} \binom{k_l}{m_{l1}, \ldots, m_{ln}, \delta_{lq}}$$

$$= \frac{(\mathbf{k} - \mathbf{1})!}{\mathbf{M}!} |\mathbf{K} - \mathbf{M}|$$

under the given conditions on $\mathbf{M}$.

The following two corollaries are, in effect, restatements of Theorem 3.1 in purely matrix terms.

COROLLARY 3.2. *Let* $\mathbf{J}$ *be the* $n \times n$ *matrix of all* 1*'s. Then*

$$\text{trace } (\mathbf{I} - \mathbf{X}\mathbf{A})^{-1}\mathbf{X}\mathbf{J} = \sum_{\mathbf{M}} \mathbf{x}^{\mathbf{k}}\mathbf{A}^{\mathbf{M}}|\mathbf{K} - \mathbf{M}|(\mathbf{k} - \mathbf{1})!(\mathbf{M}!)^{-1}$$

where the summation is taken over all non-negative integer matrices $\mathbf{M}$ *such that there exist* $p, q \in \mathscr{N}$ *for which*

$$k_j = \sum_{i=1}^{n} m_{ij} + \delta_{pj}, \; j = 1, 2, \ldots, n$$
$$k_i = \sum_{j=1}^{n} m_{ij} + \delta_{iq}, \; i = 1, 2, \ldots, n.$$

Proof. From Lemma 2.2

$$\mathbf{y}^T = \mathbf{x}^T + \mathbf{X}\mathbf{A}\mathbf{y}^T$$

so $y_i = [(\mathbf{I} - \mathbf{X}\mathbf{A})^{-1}\mathbf{X}\mathbf{J}]_{ii}$. Thus trace $(\mathbf{I} - \mathbf{X}\mathbf{A})^{-1}\mathbf{X}\mathbf{J} = y_1 + \ldots + y_n$ and the corollary follows from Theorem 3.1.

COROLLARY 3.3.

$$[(\mathbf{I} - \mathbf{X}\mathbf{A})^{-1}\mathbf{X}]_{pq} - x_q k_p \sum_{\mathbf{M}} \mathbf{x}^{\mathbf{k}}\mathbf{X}^{\mathbf{M}} \{\text{cof}_{pq}(\mathbf{K} - \mathbf{M})\} (\mathbf{k} - \mathbf{1})!(\mathbf{M}!)^{-1}$$

where the summation is taken over all non-negative integer matrices $\mathbf{M}$ *where the row sums and the column sums of* $\mathbf{K} - \mathbf{M}$ *are zero.*

Proof. $[(\mathbf{I} - \mathbf{X}\mathbf{A})^{-1}\mathbf{X}]_{pq}$ is the generating function for the subset of sequences of $\mathscr{S}^+$ which begin with p and end with q. The corollary follows from Proposition 2.1 and Theorem 3.1.

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In the following section a number of applications of these results is considered.

4. Applications. We now consider the use of these results in determining the number of Eulerian and Hamiltonian dicircuits of a directed graph.

COROLLARY 4.1 (de Bruijn-van Aardenne Ehrenfest-Smith-Tutte theorem [**1**]). *Let $\mathscr{G}$ be a digraph with vertex set $\{v_1, \ldots, v_n\}$ such that in − degree (v_i) = out − degree $(v_i) = k_i$ for $i = 1, 2, \ldots, n$. If $e(\mathscr{G})$ is the number of Eulerian dicircuits in $\mathscr{G}$ and $t_i(\mathscr{G})$ is the number of spanning arborescences of $\mathscr{G}$ rooted at v_i then*

$$e(\mathscr{G}) = (k-1)!t_i(\mathscr{G}) \text{ for } i = 1, 2, \ldots, n.$$

Proof. Consider the sequences of $\mathscr{S}^+$ which begin and end at p, and let n_{pp} be the number of such sequences. Then

$$e(\mathscr{G}) = \mathbf{M}!n_{pp}$$

since the edges are distinct. Now let $x_1 = x_2 = \ldots = x_n = 1$ in Theorem 3.1 since the information about vertices is not to be retained. Then from Theorem 3.1 we have directly

$$n_{pp} = [A^{\mathbf{M}}]y_p = |\mathbf{K} - \mathbf{M}|(\mathbf{k} - \mathbf{1})!(\mathbf{M}!)^{-1}$$

where

$$k_j = \sum_{i=1}^n m_{ij} + \delta_{pj} \text{ and}$$
$$k_i = \sum_{j=1}^n m_{ij} + \delta_{ip}.$$

Thus

$$e(\mathscr{G}) = (\mathbf{k} - \mathbf{1})!|\mathbf{K} - \mathbf{M}|.$$

But $|\mathbf{K} - \mathbf{M}| = \mathrm{cof}_{pp}(\mathbf{K} - \mathbf{M}) = \mathrm{cof}_{pp}(\mathbf{K} - \mathbf{G})$ where $\mathbf{G}$ is the adjacency matrix of $\mathscr{G}$. But

$$\mathrm{cof}_{pp}(\mathbf{K} - \mathbf{G}) = t_p(\mathscr{G})$$

by the Matrix-tree theorem ([**2**] and [**13**]) and the corollary follows.

Corollary 3.3 is a slight restatement of the result of Hutchinson and Wilf [**8**] who obtained the number of sequences in $\mathscr{S}^+$ with a prescribed set of symbols and a prescribed number of subsequences of the form ij. However, their proof invokes the de Bruijn-van Aardenne Ehrenfest-Smith-Tutte theorem while our treatment derives it.

COROLLARY 4.2. *Let $\mathscr{G}$ be a digraph on n vertices with adjacency matrix* $\mathbf{G}$. *If $h(\mathscr{G})$ is the number of Hamiltonian dicircuits in $\mathscr{G}$ then*

$$h(\mathscr{G}) = \sum_{k=0}^{n-1} (-1)^k \sum_{\alpha \subseteq \mathscr{N} \setminus \{p\}} \det \mathbf{G}[\alpha|\alpha] \operatorname{per} \mathbf{G}(\alpha|\alpha), \quad \text{for any } p \in \mathscr{N}$$

where $\mathbf{G}[\alpha|\alpha]$ *is the submatrix of* A *with rows and columns from* α *and* $\mathbf{G}(\alpha|\alpha) = \mathbf{G}[\mathscr{N}\backslash\alpha|\mathscr{N}\backslash\alpha]$.

Proof. Let $\sigma \in \mathscr{S}^+$ be a sequence beginning and ending with p, and containing each of the remaining symbols exactly once. Then each such σ corresponds to a Hamiltonian dicircuit of $\mathscr{G}$. Thus, from Lemma 2.2 we have,

$$h(\mathscr{G}) = [x_1 \ldots x_{p-1}x_p^2x_{p+1} \ldots x_n]y_p$$

where $\mathbf{y}$ satisfies

$$\mathbf{y}^T = \mathbf{x}^T + \mathbf{XGy}^T.$$

Thus $y_p = [(\mathbf{I} - \mathbf{XG})^{-1}\mathbf{X}]_{pp}$ whence

$$h(\mathscr{G}) = [x_1 \ldots x_n]\ |\mathbf{I} - \mathbf{XG}|^{-1} \operatorname{cof}_{pp}(\mathbf{I} - \mathbf{XG}).$$

But by the MacMahon Master Theorem ([**11**] and [**3**]) we have

$$[x_{\alpha_1} \ldots x_{\alpha_k}]\ |\mathbf{I} - \mathbf{XG}|^{-1} = \operatorname{per} \mathbf{G}[\alpha|\alpha]$$

where $\alpha = \{\alpha_1, \ldots, \alpha_k\} \subseteq \mathscr{N}$.
Accordingly

$$|\mathbf{I} - \mathbf{XG}|^{-1} = \sum_{k=0}^{n} \sum_{\substack{\alpha \subseteq \mathscr{N} \\ |\alpha|=k}} x_{\alpha_1} \ldots x_{\alpha_k} \operatorname{per} \mathbf{G}[\alpha|\alpha] + F(\mathbf{x})$$

where $F(\mathbf{x})$ consists of the remaining terms, each of which contains an x_i to a power greater than one. But, expanding the determinant of the sum of a pair of matrices [**12**],

$$\operatorname{cof}_{pp}(\mathbf{I} - \mathbf{XG}) = \sum_{l=0}^{n-1} (-1)^l \sum_{\substack{\beta \subseteq \mathscr{N}\backslash\{p\} \\ |\beta|=l}} x_{\beta_1} \ldots x_{\beta_l} \det \mathbf{G}[\beta|\beta].$$

Thus

$$h(\mathscr{G}) = [x_1 \ldots x_n] \sum_{k,\,l} (-1)^l \sum_{\substack{\alpha \subseteq \mathscr{N} \\ |\alpha|=k}} \sum_{\substack{\beta \subseteq \mathscr{N}\backslash\{p\} \\ |\beta|=l}} \times x_{\alpha_1} \ldots x_{\alpha_k} x_{\beta_1} \ldots x_{\beta_l} \operatorname{per} \mathbf{G}[\alpha|\alpha] \det \mathbf{G}[\beta|\beta]$$

and the theorem follows.

This expression for $h(\mathscr{G})$ involves the sum over all subsets of $\mathscr{N}\backslash\{p\}$. It is rather more efficient than the expression given by [**15**], for Hamiltonian circuits, which involves a sum over all partitions of $\mathscr{N}$.

5. Concluding remarks. Hutchinson and Wilf have considered the situation in which **A** is symmetric and have reported that they encountered considerable difficulties [**8**]. Unfortunately, analogous difficulties present themselves in the application of the methods of the proof of Theorem 3.1, for in this case the partial derivatives with respect to a_{ij} contain more terms than in the case we have treated. We have been unable to detect any elegant simplifications which would warrant a disclosure. It would appear that the reason why the proof of Theorem 3.1 may be carried out is that $f_i(\mathbf{y})$ is linear in $a_{i1}, \ldots, a_{in}$ and $y_1, \ldots, y_n$. Indeed, any departure at all from these serious constraints appears to lead either to a situation in which the Lagrange theorem cannot be applied or to an intolerable proliferation of terms which do not condense. For example, an expansion of trace $(\mathbf{I} - \mathbf{XAX}(\mathbf{J} - \mathbf{A}))^{-1}\mathbf{XJ}$, which enumerates general alternating sequences [**10**] remains intractable by this method in spite of the apparent close affinity of this expression to trace $(\mathbf{I} - \mathbf{XA})^{-1}\mathbf{XJ}$, which appears in the statement of Corollary 3.2.

It is interesting, although not altogether surprising, that at the other extreme, where $\mathbf{A}$ has the form

$$a_{ij} = \begin{cases} y \text{ if } i < j \\ z \text{ if } i = j \\ x \text{ if } i > j \end{cases}$$

so that the elements of $\mathbf{A}$ are highly dependent, the generating function $\Phi(\mathbf{x}, \mathbf{A})$ again may be determined [**8**]. This fact unifies a large number of well known sequence enumeration problems under a common approach.

A number of applications of the multivariate Lagrange theorem and the de Bruijn—van Aardenne Ehrenfest—Smith—Tutte theorem to sequence enumeration may be found in [**4**], [**6**] and [**7**].

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