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COUNTING LABELLED TREES

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FOREWORD

La publication de la conférence de John Moon, *Counting Labelled Trees*, est un autre jalon de l'histoire de la Société Mathématique du Canada. Nous espérons que cette monographie sera la première d'une longue série.

Du point de vue historique, les premières publications de la Société ont été limitées aux comptes rendus des Congrès et peu après au Journal Canadien de Mathématiques. Dans les premiers temps, la publication du Journal Canadien était une entreprise d'envergure et avait tendance à prendre le pas sur les autres efforts de publication. Avec l'avènement du Bulletin Canadien de Mathématiques, les autres publications ont été pour ainsi dire négligées. Ce fait est à déplorer si l'on considère la haute valeur d'un grand nombre des conférences de nos séminaires. Plusieurs de ces conférences furent publiées sous forme de notes polycopiées qui, en plus de n'être pas très attrayantes, n'étaient à la disposition que d'un petit nombre. De fait, elles auraient mérité une meilleure diffusion - réalisable si ces notes avaient paru sous forme de livre.

La société se considère privilégiée de pouvoir commencer cette série avec une oeuvre de John Moon. Avec la compétence qui le caractérise il a su réunir les éléments d'un sujet intéressant et de lecture très agréable.

En tant que président de la Société Mathématique du Canada, je désire offrir mes félicitations au professeur Moon qui lance cette série et établit ainsi un haut degré d'excellence que ses successeurs voudront atteindre.

N. S. Mendelsohn

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The publication of John Moon's *Counting Labelled Trees* marks yet another milestone in the history of the Canadian Mathematical Congress. It is hoped that this monograph will be the first of a continuing series.

Historically, the early publications of Congress were confined to the *Proceedings of Congresses* and shortly after that the *Canadian Journal of Mathematics*. In those first days the publication of the Canadian Journal was a large undertaking and tended to push into the background other efforts of publication. With the coming of the *Canadian Mathematical Bulletin*, other publications were virtually neglected. In retrospect, this is a great pity since such activities as our biennial seminars contained a large number of magnificent lecture series. Many of these appeared as mimeographed lecture notes which, besides their unattractive appearance, were available only to a few. In fact, they deserved widespread circulation and this would have been achieved if the notes had been edited and published in book form.

Congress is very fortunate in having the first book of this series written by John Moon. With impeccable scholarship, he has put together the results of an attractive subject in a highly readable form.

As president of the Canadian Mathematical Congress, I wish to congratulate Professor Moon for launching the series and setting a high standard for others to follow.

N. S. Mendelsohn

My object has been to gather together various combinatorial results on labelled trees. The basic definitions are given in the first chapter; enumerative results are presented in the next five chapters, classified according to the type of argument involved; some probabilistic problems on random trees are treated in the last chapter. Some familiarity with matrices and generating functions is presupposed, in places, but much of the exposition should be accessible to anyone who knows something about finite mathematics or probability theory.

This material was originally prepared for a series of lectures I gave at the Twelfth Biennial Seminar of the Canadian Mathematical Congress at the University of British Columbia in August, 1969. I am indebted to Professors Ronald Pyke and John J. McNamee for their invitation and encouragement.

Edmonton, Alberta February, 1970 J. W. M.

1.	Intr	oduction	rage
ец. 1615	1.1	Definitions	1
	1.2	Properties of Trees	1
	1.3	Summary	3
1	Ass	relating Sequences with Trees	
रहर	2.1	Priifer Sequences	4
45 1.50	2.2	Tree Functions	. 6
ৰ্মান জন্ম	2.3	Knuth's Generalization of Prüfer Sequences	7
	2.4	Special Cases	8
3.	Indu	ictive Arguments	
C_{λ}	3.1	Some Identities	12
	3.2	Trees with a Given Degree Sequence	13
${\rm d}_{{\rm e}_{i}}$	3.3	Trees in which the Degree of a Given Node is Specified	14
67	3.4	The Number of k-Trees	16
5.0	3.5	Forests of Trees with Specified Roots	17
1	3.6	Connected Graphs with One Cycle	19
	3.7	Trees with a Given Number of Endnodes	20
	3.8	Recurrence Relations for $T(n)$	21
	3.9	Connected Graphs with Unlabelled Endnodes	23
4.	Арр	lications of Generating Functions	
	4.1	Counting Connected Graphs	25
	4.2	Counting Rooted Trees and Forests	26
	4.3	Counting Unrooted Trees and Forests	27
1	•		/ i
			14

Page

CONTENTS

* ... e Nes

1.

Ś

x	Co	ontents	
	4.4	Bipartite Trees and Forests	30
	4.5	Counting Trees by Number of Inversions	32
	4.6	Connected Graphs with Given Blocks	33
5.	The	Matrix Tree Theorem	
	5.1	Introduction	39
	5.2	The Incidence Matrix of a Graph	39
	5.3	The Matrix Tree Theorem	41
	5.4	Applications	43
	5.5	The Matrix Tree Theorem for Directed Graphs	46
	5.6	Trees in the Arc-Graph of a Directed Graph	48
	5.7	Listing the Trees in a Graph	51
6.	The	Method of Inclusion and Exclusion	
	6.1	Introduction	52
	6.2	The Number of Trees Spanned by a Given Forest	52
	6.3	The Number of Spanning Trees of a Graph	54
	6.4	Examples	54
	6.5	Trees Containing a Given Number of Specified Edges	62
	6.6	Miscellaneous Results	64
7.	Pro	olems on Random Trees	
	7.1	Random Mapping Functions	66
	7.2	The Degrees of the Nodes in Random Trees	70
	7.3	The Distance between Nodes in Random Trees	76
	7.4	Trees with Given Height and Diameter	78
	7.5	The First Two Moments of the Complexity of a Graph	79
	7.6	Removing Edges from Random Trees	83
	7.7	Climbing Random Trees	86
	7.8	Cutting Down Random Trees	90
	Ref	prences	99
	Aut	nor Index	109
	Sub	iect Index	112

INTRODUCTION

1.1. Definitions. A graph G_n consists of a finite set of *n* nodes some pairs of which are joined by a single *edge*; we usually assume the nodes are labelled 1, 2, ..., *n* and that no edge joins a node with itself. A node and an edge are *incident* if the edge joins the node to another node. The *degree* of a node is the number of edges incident with it; an *endnode* of a graph is a node of degree one.

Suppose the graphs G_n and H_n have the same number of nodes. If nodes i and j of G_n are joined by an edge if and only if nodes i and j of H_n are joined by an edge, then we say G_n and H_n determine the same *labelled* graph; more generally, if G_n and H_n determine the same labelled graph for some relabelling of their nodes, then we say G_n and H_n are *isomorphic* or that they determine the same *unlabelled* graph. The labelled graphs with three nodes and the unlabelled graphs with four nodes are shown in Figures 1 and 2.

A path is a sequence of edges of the type ab, bc, cd, \ldots, lm where each edge *ij* joins the nodes *i* and *j*. We usually assume the nodes *a*, *b*, ..., *l* are distinct; if a = m we call the path a *cycle*. The *length* of a path or cycle is the number of edges it contains; sometimes it is convenient to consider a single node as a path of length zero. A graph is *connected* if every pair of nodes is joined by a path; any graph is the union of its connected *components*. The *distance* between two nodes in a connected graph is the length of any shortest path joining them.

1.2. Properties of Trees. A *tree* is a connected graph that has no cycles. König (1937; pp. 47–48) lists some of the early works in which the concept of a tree appears; the earliest were by Kirchhoff and von Staudt in 1847.

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The trees with up to six nodes and the number of ways of labelling their nodes are illustrated in Figure 3. The trees with up to ten nodes (and up to twelve nodes in some cases) were drawn by Harary and Prins (1959).



We shall use the following properties of a tree in what follows (these properties and others can be combined to provide at least sixteen equivalent definitions of a tree; see Anderson and Harary (1967) and Harary and Manvel (1968)).

LEMMA 1.1. If a tree has at least two nodes, then it has at least two endnodes.

This may be proved by considering two nodes joined by one of the longest paths in the tree.

LEMMA 1.2. If a tree has n nodes, then it has n - 1 edges.

This may be proved by induction on n, using Lemma 1.1.

LEMMA 1.3. Any two nodes of a tree are joined by a unique path.

Any two nodes of a tree must be joined by at least one path because a tree is connected; if they were joined by more than one path the tree would contain a cycle and this is impossible by definition.

1.3. Summary. Let T(n) denote the number of trees T_n with *n* labelled nodes, for n = 1, 2, ... The formula $T(n) = n^{n-2}$ is usually attributed to Cayley (1889). He pointed out, however, that an equivalent result was proved earlier by Borchardt (1860); this result appeared without proof in an even earlier paper by Sylvester (1857). The formula for the number of labelled trees has been rediscovered, conjectured, proved, and generalized many times. Our object here is to summarize various results of a combinatorial or probabilistic nature that are known about labelled trees and to survey the more important methods that have been used to establish these results. For additional material on these and related problems see, for example, Riordan (1958) and Knuth (1968a).

ASSOCIATING SEQUENCES

WITH TREES

2.1. Prüfer Sequences. Some enumeration problems for trees can be treated by associating certain sequences with trees; a useful feature of this type of argument is that various properties of the trees are reflected in the corresponding sequences.

THEOREM 2.1. If $n \ge 3$ there is a one-to-one correspondence between the trees T_n with n labelled nodes and the n^{n-2} sequences $(a_1, a_2, \ldots, a_{n-2})$ that can be formed from the numbers $1, 2, \ldots, n$.

Cayley would prove this when n = 5 by classifying the terms in a certain expansion as follows (the symbols α , β , γ , δ , and ϵ denote the numbers 1, 2, 3, 4, and 5 in some order):

$$\begin{array}{c} (\alpha + \beta + \gamma + \delta + \epsilon)^3 \alpha \beta \gamma \delta \epsilon = +3\alpha^2 \beta & 20 \\ +6\alpha \beta \gamma & 10 \end{array} \right\} \begin{array}{c} 5 \\ \alpha \beta \gamma \delta \epsilon & 60 \\ \hline 60 \\ \hline 125 \end{array}$$

The multinomial coefficients 1, 3, and 6 show how many times these terms appear, and the numbers 5, 20, and 10 show how many terms like these can be formed with the factors α , β , γ , δ , and ϵ . The terms of the type $\alpha^4 \beta \gamma \delta \epsilon = (\alpha \beta)(\alpha \gamma)(\alpha \delta)(\alpha \epsilon)$ correspond to the trees T_5 that have a node α of degree four; the terms $\alpha^3\beta^2\gamma\delta\epsilon$ correspond to the trees T_5 with a node α of degree three joined to a node β of degree two; the terms $\alpha^2 \beta^2 \gamma^2 \delta \epsilon$ correspond to the paths on five nodes with endnodes δ and ϵ .

Cayley gives no explicit rule for establishing the correspondence between trees and sequences in general. He merely exhibits such a correspondence 4

when n = 6 and remarks that "... it will be at once seen that the proof given for this particular case is applicable for any value whatever of n".

Prüfer (1918), apparently unaware of Cayley's paper, constructs the correspondence as follows. From any tree T_n remove the endnode (and its incident edge) with the smallest label to form a smaller tree T_{n-1} and let a_1 denote the (label of the) node that was joined to the removed node; repeat this process on T_{n-1} to determine a_2 and continue until only two nodes, joined by an edge, are left. The tree in Figure 4, for example, determines the sequence (2, 8, 6, 2, 8, 2). Different trees T_n determine





different sequences $(a_1, a_2, \ldots, a_{n-2})$; it remains to show that each such sequence corresponds to some tree T_n .

Suppose $(a_1, a_2, \ldots, a_{n-2})$ is any sequence formed from the numbers 1, 2, ..., n. If b_1 denotes the smallest positive integer that does not occur in the sequence, let (c_2, \ldots, c_{n-2}) denote the sequence obtained from (a_2, \ldots, a_{n-2}) by diminishing all terms larger than b_1 by one. Then (c_2, \ldots, c_{n-2}) is a sequence of length n-3 formed from the numbers 1, 2, ..., n-1 and we may assume there exists a tree T_{n-1} with nodes 1, 2, ..., n-1 that corresponds to this sequence. Relabel the nodes of T_{n-1} by adding one to each label that is not less than b_1 ; if we introduce an *n*th node labelled b_1 and join it to the node labelled a_1 in T_{n-1} , we obtain a tree T_n that corresponds to the original sequence $(a_1, a_2, \ldots, a_{n-2})$. This shows that Prüfer's construction provides a one-to-one correspondence between these sequences and the trees T_n .

Neville (1953) gives three methods for defining a sequence corresponding to a tree (see also Knuth (1968a; p. 397)). The first is the method just described. The second differs in that if we have just removed a node b_i that was joined to a_i we remove a_i next if a_i is now an endnode; otherwise we remove the endnode with the smallest label as before. In the third method all the endnodes of the original tree are removed in the order of the size of their labels; then all the endnodes of the remaining tree are removed, and so on. The sequences $(a_1, a_2, \ldots, a_{n-2})$ are defined in terms of the nodes removed as before. The tree in Figure 4, for example, determines the sequences (2, 8, 6, 8, 2, 2) and (2, 8, 6, 2, 2, 8) if these last two methods are used. It can be shown by modifications of the argument given earlier that each sequence $(a_1, a_2, \ldots, a_{n-2})$ corresponds to some tree T_n with respect

to these methods. (The last two methods described are not quite the same as the methods described by Neville; he would never remove the node labelled n.)

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It is not difficult to see that if node *i* of T_n has degree d_i , then the number *i* occurs $d_i - 1$ times in the sequence associated with T_n (this is true no matter which of the three methods for constructing the sequence is used). Since any sequence $(a_1, a_2, \ldots, a_{n-2})$ formed from the numbers $1, 2, \ldots, n$ determines a tree T_n , it follows that the only restriction on the d_i 's is that they be positive integers and that $\sum_{i=1}^{n} (d_i - 1) = n - 2$. Thus the positive integers (d_1, d_2, \ldots, d_n) form the *degree sequence* of some tree T_n if and only if their sum is 2(n - 1). This result apparently first appears in a paper by Senior (1951) as a special case of a more general result (see also Bäbler (1953), Hakimi (1962), Menon (1964), and Ramanujacharyulu (1965)). It also follows from Prüfer's construction that the number of trees T_n with a given degree sequence (d_1, d_2, \ldots, d_n) is given by the multinomial coefficient

(2.1)
$$\begin{pmatrix} n-2\\ d_1-1,\ldots,d_n-1 \end{pmatrix}$$

This formula, which was pointed out by Moon (1964, 1967a) and Riordan (1966), can be used to derive a number of other results as we shall see later. (Zarankiewicz (1946) has pointed out that if a tree has p endnodes and q nodes whose degree exceeds two, then the sum of the degrees of these latter q nodes equals 2(q - 1) + p.)

2.2 Tree Functions. Before describing some extensions of Prüfer's method we introduce more terminology. Suppose we choose some specific node of a tree T_n , say the *n*th node, and call it the *root*. There exists a unique path from any other node *i* to the root; if *ij* is the first edge in this path let f(i) = j. The function *f* is called the *tree function* of T_n . We could represent the function *f* by the *directed rooted tree*—sometimes called an *arborescence*—obtained from T_n by replacing each edge *ij* by an arc *ij* directed from *i* to *j*, where j = f(i); each node, with the exception of the root, now has exactly one arc directed away from it. Suppose *f* is any function that maps $\{1, 2, \ldots, n-1\}$ into $\{1, 2, \ldots, n\}$. Glicksman (1963) has shown that *f* is a tree function if and only if $\{f(i): i \in A\} \notin A$ for every non-empty subset *A* of $\{1, 2, \ldots, n-1\}$. The necessity of this condition follows from the fact that a tree has no cycles; the sufficiency can be proved by constructing a tree that corresponds to *f* by working backwards inductively from the root.

A. Lempel, E. Palmer, and perhaps others have observed that there are n^{n-3} different trees with *n* unlabelled nodes and n-1 edges labelled 1, 2, ..., n-1 when $n \ge 3$. One way to prove this is as follows. Let *f*

denote the tree function of a node-labelled tree T_n ; assign the label *i* to the edge *ij*, where j = f(i), for i = 1, 2, ..., n - 1. It is not difficult to see that this defines a mapping of the set of n^{n-2} node-labelled trees T_n onto the set of edge-labelled trees and, when $n \ge 3$, each edge-labelled tree is the image of *n* node-labelled trees. Palmer (1969) has treated similar problems for a different type of tree.

We digress a moment to mention the following problem of Riordan's, although perhaps it is not obvious that the problem has anything to do with trees. There are *n* parking spaces available along a street and each of *n* drivers, arriving consecutively, has a preferred parking space; the *i*th driver will park in space g(i) if it is still available when he arrives and if it is not he will park in the next unoccupied space he finds (if there is one). Every driver can find a parking space (without driving around the block) if there exists a permutation π of $\{1, 2, \ldots, n\}$ such that $\pi(j)$ is the least integer greater than or equal to g(j) that is not in the set $\{\pi(1), \ldots, \pi(j-1)\}$ for $1 \le j \le n$. Schützenberger (1968) showed by induction that there is a one-to-one correspondence between the preference functions g in which everyone finds a parking space and the tree functions that map $\{1, 2, \ldots, n\}$ into $\{1, 2, \ldots, n + 1\}$. Riordan (1969) has given other more direct proofs of the fact that there are $(n + 1)^{n-1}$ such functions g.

2.3. Knuth's Generalization of Prüfer Sequences. A directed graph D consists of a collection of nodes some ordered pairs of which are joined by a directed edge, or *arc*; we say the arc ij is directed from node *i* to node *j*. The graph D may contain both of the arcs ij and ji and it may contain arcs of the type ii called *loops*.

A graph is a *spanning* subgraph of a second graph if they have the same nodes and every edge (or arc) in the first graph is also in the second. When we refer to a spanning subtree of a directed graph, we shall always mean a directed rooted tree of the type described above in which each arc is directed towards the root; in particular, if the directed graph is rooted at a particular node x, then the spanning subtree is to be rooted at x.

If D is any directed graph with h labelled nodes and (s_1, s_2, \ldots, s_h) is any composition of n into h positive integers, let H denote the graph obtained by replacing each node i of D by a set S_i of s_i nodes; the arc \overrightarrow{xy} is in H if and only if x and y belong to subsets S_i and S_j such that the arc \overrightarrow{ij} was in D. (Notice that if D had some loops, then H also has loops.) We assume for convenience that the n nodes are labelled so that if i < j then the nodes of S_i have smaller labels than the nodes of S_j . We also assume $S_h = 1$ so S_h consists simply of the nth node; we think of this node as the root of both D and H although it is labelled differently in the two graphs.

Let $\Gamma(S_i)$ denote the set of nodes y in H such that y is the terminal node

8 Associating Sequences with Trees

of some arc issuing from a node of S_i (notice that $S_i \subseteq \Gamma(S_i)$ if the loop \vec{ii} is in D). If f is the tree function of a spanning subtree of G (that is rooted at the hth node of G), let $f(S_i) = S_j$ if j = f(i) for i = 1, 2, ..., h - 1. We shall let |X| denote the number of elements in the set X.

The following result is a special case of a more general result due to Knuth (1968); it expresses the number c(H) of spanning subtrees of H (rooted at node n) in terms of the spanning subtrees of D (rooted at node h).

THEOREM 2.2. If $h \ge 2$, then

$$c(H) = \sum_{f} \left\{ \prod_{i=1}^{h-1} |\Gamma(S_i)|^{s_i-1} \cdot |f(S_i)| \right\},$$

where the sum is over the tree functions f of all spanning subtrees of D.

The proof involves showing there is a one-to-one correspondence between trees spanning H and the ordered sets of h - 1 sequences of the form

$(a(i, 1), a(i, 2), \ldots, a(i, s_i)),$

where a(i, j) is any member of $\Gamma(S_i)$ for $j = 1, 2, ..., s_i - 1$, and $a(i, s_i)$ is any member of $f(S_i)$, for i = 1, 2, ..., h - 1, for the tree function f of some spanning subtree of D.

Suppose the tree T spans the graph H. We successively remove the endnodes with the smallest labels, as before; now, however, when we remove an endnode b from a subset S_i we write the label of the node joined to b in the next position of the *i*th sequence. When only one edge remains, joining some node of S_j , say, to the *n*th node, we put an n in the last position of the *j*th sequence. It is clear that each term a(i, j) belongs to $\Gamma(S_i)$. When the last node b of S_i is removed, suppose the node joined to b belongs to the subset S_j . If we let f(i) = j, then it is not difficult to show, using Glicksman's result, that the function f is the tree function of a spanning subtree of D. Thus, every tree spanning H can be associated with a set of sequences of the type described above. It can be shown by induction that there exists a spanning tree of H corresponding to each such set of sequences.

Knuth's more general result applies when $s_h \ge 1$ and one wants to determine the number of families of disjoint directed rooted trees that collectively span H and whose roots constitute specified subsets of nodes of H; we now describe three corollaries he deduced from his theorem.

2.4. Special Cases. Suppose the graph H is obtained from the directed graph D illustrated in Figure 5. There is only one spanning subtree of D



(rooted at the bottom node) and its arcs are $\vec{12}$, $\vec{23}$, and $\vec{34}$. It follows from Theorem 2.2 that there are $s_2^{s_1}s_3^{s_2}(s_1 + 1)^{s_3-1}$ spanning subtrees of H. If we think of the bottom node as a member of S_1 , then we can think of H as having arisen from a directed 3-cycle and we can abandon the restriction $s_h = 1$. The following more general result can be proved in the same way.

COROLLARY 2.2.1. If the graph D is a directed h-cycle and $h \ge 2$, then there are

$$s_2^{s_1-1}s_3^{s_2}\cdots s_h^{s_{h-1}}s_1^{s_h-1}$$

spanning subtrees of H that are rooted at any given node of the first subset of nodes.

Theorem 2.2 also applies when the graphs D and H are ordinary undirected graphs since any undirected graph G can be transferred into an equivalent directed graph D by replacing each edge ij by the arcs ij and ji. The following result, apparently proved first by Rohličkova (1966) by another method, is the analogue of Corollary 2.2.1 for ordinary undirected graphs.

COROLLARY 2.2.2. If G is a cycle of length $h(\geq 2)$, then

$$c(H) = (s_h + s_2)^{s_1 - 1} (s_1 + s_3)^{s_2 - 1} \cdots (s_{h-1} + s_1)^{s_h - 1} s_1 s_2 \cdots s_h \\ \times ((s_1 s_2)^{-1} + (s_2 s_3)^{-1} + \cdots + (s_h s_1)^{-1}).$$

To prove this we select some node to serve as a root, treat it as though it constituted a separate subset by itself, and apply Theorem 2.2 as before; the details of the derivation are somewhat more complicated than they were in the proof of Corollary 2.2.1, however, because the root-node is joined to nodes from two other subsets of nodes of H and there are more spanning subtrees to consider.

If the (undirected) graph G is a tree with h nodes, there is only one spanning subtree of G, namely G itself. There is no loss of generality if we assume the hth node is an endnode. If we ignore the restriction $s_h = 1$ and treat some node in the hth subset of nodes of H as a root-node constituting a separate subset by itself, we find that the formula in Theorem

10 Associating Sequences with Trees

2.2 can be rewritten as follows. (The result still holds even if G has some loops if they are ignored in determining the degree sequence.)

COROLLARY 2.2.3. If G is a tree with degree sequence (d_1, d_2, \ldots, d_h) , then

$$c(H) = \prod_{i=1}^{h} |\Gamma(S_i)|^{s_i - 1} s_i^{d_i - 1}$$

An r by s bipartite graph is a graph with r "dark" nodes and s "light" nodes such that every edge of the graph joins a dark node with a light node. If we let G be the graph consisting of a single edge joining two nodes, then it follows from Corollary 2.2.3 (or 2.2.1) that there are $r^{s-1}s^{r-1}$ bipartite trees with r labelled dark nodes and s labelled light nodes. This particular result was apparently first proved by Fiedler and Sedláček (1958); we shall discuss their derivation and others later. If (r_1, \ldots, r_r) and (s_1, \ldots, s_s) are compositions of r + s - 1 into positive integers, then it follows from the proof of Theorem 2.2 that there are

(2.2)
$$\binom{s-1}{r_1-1,\ldots,r_r-1} \cdot \binom{r-1}{s_1-1,\ldots,s_s-1}$$

bipartite trees for which the degree sequences of the r dark nodes and the s light nodes are (r_1, \ldots, r_r) and (s_1, \ldots, s_s) . This formula can be used to derive the following results of Klee and Witzgall (1967); if s = ru + 1 then there are $(ru + 1)^{r-1}(ru)!/(u!)^r r$ by s trees in which the r dark nodes all have degree u + 1; if s = ru - 1 then there are $r^{r-2}(ur - 1)!/((u - 1)!)^r$ r by s trees in which u - 1 of the nodes joined to each dark node are endnodes.

Every tree T_n corresponds to two r by s bipartite trees, for some values of r and s (if we think of the nth node as belonging to one of the two node sets then the *i*th node will belong to the same node set or the other node set according as the distance between *i* and n in T_n is even or odd). It follows from this observation that

$$\sum_{k=0}^{n} {n \choose k} k^{n-k-1} (n-k)^{k-1} = 2n^{n-2};$$

this is a special case of the second identity listed later in Table 1 and Austin (1960) has derived a multinomial extension of this identity.

The proof of Theorem 2.2 also yields a solution to a problem considered by Raney (1964) in the course of deriving a formal power series solution to the equation $\sum_{i=1}^{\infty} A_i \exp(B_i X) = X$. Let *B* denote some subset of *k* nodes of a subset *A* of *n* labelled nodes; let $c = (c_1, \ldots, c_t)$ and e = (e_1, \ldots, e_t) denote compositions of *n* and n - k into *t* non-negative integers. Let T(n, k; c, e) denote the number of *forests F* of *k* disjoint rooted trees that can be formed on the nodes of A subject to the following conditions: (1) each tree T in the forest F contains just one node of B and this node is the root of T; (2) each node of A is assigned one of t colours and there are c_i nodes of the *i*th colour; and (3) each edge in a tree T of F is given the same colour as the node with which it is incident that is nearest the root of T and there are e_i edges of the *i*th colour in F.

COROLLARY 2.2.4.

$$T(n,k;c,e)=\frac{k}{n}\binom{n}{c_1,\ldots,c_t}\binom{n-k}{e_1,\ldots,e_t}c_1^{e_1}\cdots c_t^{e_t}.$$

Let G denote the graph on three nodes in which the second node is joined to the first and third nodes; the first node is also joined to itself by a loop. Let H be the graph defined earlier with h = 3 and $(s_1, s_2, s_3) = (n - k, k, 1)$; we consider the nodes of S_2 as the nodes of B and the nodes of S_1 as the remaining nodes of A. It follows from the proof of Theorem 2.2 that each spanning subtree of H corresponds to a pair of sequences

$$(a_1, a_2, \ldots, a_{n-k})$$
 and (b_1, b_2, \ldots, b_k) ,

where $a_i \in S_1 \cup S_2$ for i = 1, 2, ..., n - k - 1, $a_{n-k} \in S_2$, $b_i \in S_1 \cup \{n + 1\}$ for i = 1, 2, ..., k - 1, and $b_k = n + 1$. It is not difficult to see that forests F on the nodes of $A = S_1 \cup S_2$ consisting of k disjoint rooted trees each of which is rooted at a node of $B = S_2$ correspond to spanning subtrees of H in which the (fictitious) (n + 1)st node is joined to every node of B; such subtrees correspond to the sequences in which $b_i = n + 1$ for i = 1, 2, ..., k. It remains to enumerate the sequences $(a_1, a_2, ..., a_{n-k})$ corresponding to forests F satisfying conditions (2) and (3) also.

There are $\binom{n}{c_1, \ldots, c_t}$ ways to colour the nodes of A and satisfy condition (2). Once this has been done, there must be e_i positions in the sequence $(a_1, a_2, \ldots, a_{n-k})$ in which the label of one of the c_i nodes of colour *i* appears. These positions can be chosen and filled in

$$\binom{n-k}{e_1,\ldots,e_t}c_1^{e_1}\cdots c_t^{e_t}$$

ways. Of all the possible sequences thus constructed only the fraction k/n have the additional property that $a_{n-k} \in S_2 = B$ and thus correspond to suitable forests F. This completes the proof of the corollary. If t = 1, then the above formula reduces to kn^{n-k-1} ; this particular result was also stated by Cayley and, implicitly, by Borchardt.

INDUCTIVE ARGUMENTS

3

3.1. Some Identities. Various formulas for the number of trees enjoying certain properties can be established by induction; such arguments usually require a knowledge of an appropriate identity or recurrence relation.

Riordan (1968, Section 1.5) has given an elementary derivation of a number of identities involving Abel sums of the type

$$A_n(x, y; p, q) = \sum_{k=0}^n \binom{n}{k} (x+k)^{k+p} (y+n-k)^{n-k+q}$$

In what follows we shall make use of some special cases of the identities listed in the following table.

TABLE 1

p	q	$A_n(x, y; p, q)$
-1	0	$x^{-1}(x+y+n)^n$
-1	-1	$(x^{-1} + y^{-1})(x + y + n)^{n-1}$
1	-1	$y^{-1}(x + y + n + \beta(x))^n$
2	-1	$y^{-1}\{(x + y + n + \beta(x; 2))^n + (x + y + n + \alpha + \gamma(x))^n\}$
The	conve	ention is adopted that
		$\alpha^k \equiv \alpha_k = k!, \qquad \beta^k(x) \equiv \beta_k(x) = k! (x + k),$
		$[\beta(x; 2)]^{k} \equiv \beta_{k}(x; 2) = [\beta(x) + \beta(x)]^{k},$

and

$$\gamma^k(x) \equiv \gamma_k(x) = k \cdot k! (x + k)$$

3.2. Trees with a Given Degree Sequence. We saw earlier that formula (2.1) for the number $T(n; d_1, d_2, \ldots, d_n)$ of trees T_n whose degree sequence is (d_1, d_2, \ldots, d_n) could be deduced from Prüfer's argument. The following derivation, given by Moon (1967b), is based on the fact that the multinomial coefficients satisfy the recurrence relation

(3.1)
$$\binom{m}{a_1, a_2, \ldots, a_i} = \sum \binom{m-1}{a_1, \ldots, a_i - 1, \ldots, a_i},$$

where the sum is over all *i* such that $a_i \ge 1$.

THEOREM 3.1. If $n \ge 3$, then

$$T(n; d_1, d_2, \ldots, d_n) = {n-2 \choose d_1 - 1, \ldots, d_n - 1}.$$

We may suppose that (d_1, d_2, \ldots, d_n) is a composition of 2(n - 1) into positive integers since $T(n; d_1, d_2, \ldots, d_n) = 0$ otherwise. It will simplify the notation later if we assume that $d_n = 1$ (this is no real loss of generality since some nodes must be joined to only one other node). We now show that

(3.2)
$$T(n; d_1, d_2, \ldots, d_n) = \sum T(n-1; d_1, \ldots, d_i - 1, \ldots, d_{n-1}),$$

where the sum is over all *i* such that $d_i \ge 2$.

Consider any tree T_n with degree sequence (d_1, d_2, \ldots, d_n) where the *n*th node is joined only to one other node, say the *i*th; it must be that $d_i \ge 2$ if $n \ge 3$ since the tree is connected. If the *n*th node is removed (along with its incident edge), then the remaining tree T_{n-1} has degree sequence $(d_1, \ldots, d_i - 1, \ldots, d_{n-1})$. This process is reversible and equation (3.2) follows upon considering all possible values of *i*. The theorem now follows from (3.1) and (3.2) by induction since it certainly holds when n = 3. Let

$$C_n = C_n(X_1, \ldots, X_n) = \sum X_1^{d_1(T)-1} \cdots X_n^{d_n(T)-1}$$

where the sum is over all trees T with n labelled nodes and $d_i(T)$ denotes the degree of the *i*th node of T. Rényi (1970) shows that

$$C_n(X_1,\ldots,X_{n-1},0) = (X_1 + \cdots + X_{n-1})C_{n-1}(X_1,\ldots,X_{n-1}),$$

by essentially the same argument as we used to establish (3.2). He then deduces that $C_n(X_1, \ldots, X_n) = (X_1 + \cdots + X_n)^{n-2}$ by applying induction and appealing to the fact that C_n is a symmetric polynomial in its *n* variables and is homogeneous of degree n - 2; he suggests that this may have been the argument Cayley originally had in mind.

14 Inductive Arguments

An oriented tree is a tree in which each edge ij is replaced by one (and only one) of the arcs ij or ji. The out-degree w_i and in-degree l_i of the *i*th node is the number of arcs of the type ij and ji, respectively, in the tree. Let (w_1, \ldots, w_n) and (l_1, \ldots, l_n) be two compositions of n - 1 into non-negative integers such that $w_i + l_i \ge 1$ for each *i*. Menon (1964) proved that these conditions are necessary and sufficient for there to exist an oriented tree T_n whose *i*th node has out-degree w_i and in-degree l_i for $i = 1, 2, \ldots, n$. The argument used to prove Theorem 3.1 can be extended to show that there are

$$\binom{n-2}{w_1+l_1-1,\ldots,w_n+l_n-1}$$

such trees.

3.3. Trees in which the Degree of a Given Node is Specified. Let C(n, k) denote the number of trees T_n in which a given node, say the *n*th, has degree $d_n = k$. The following result is due to Clarke (1958).

THEOREM 3.2. If
$$1 \le k \le n-1$$
, then $C(n,k) = \binom{n-2}{k-1}(n-1)^{n-k-1}$.

Let R_n denote any tree in which $d_n = k - 1$ and suppose we remove one of the n - k edges *ij* not incident with the *n*th node. If f(i) = j, where *f* is the tree function of R_n , then if we join the *n*th and *i*th nodes by an edge we obtain a tree T_n in which $d_n = k$. The same tree T_n could, however, be obtained from different trees R_n in this way.

If we were to remove the *n*th node (and its k incident edges) from T_n , the graph remaining would be forest of k subtrees. We can transform T_n back into a tree R_n in which $d_n = k - 1$ by replacing any edge of the type nj by an edge jl, where l and j do not belong to the same subtree. If there are n_i nodes in the *i*th subtree, then there are

$$(n-1-n_1) + \cdots + (n-1-n_k) = k(n-1) - (n-1)$$

= $(k-1)(n-1)$

ways of doing this. If we count in two ways the number of ordered pairs of trees R_n and T_n that can be transformed into each other in this way, we obtain the recurrence relation

(n-k)C(n, k-1) = (k-1)(n-1)C(n, k) for k = 2, 3, ..., n-1.

The theorem now follows by induction on (decreasing) k since

$$C(n,n-1)=1.$$

The formula for C(n, k) also follows from Theorem 3.1 and from Prüfer's construction (see Bedrosian (1964)); de Bruijn (1964) posed the formula as a problem. Klee and Witzgall (1967) used Clarke's method to show that there are

(3.3)
$$r^{s-1}\binom{r-1}{k-1}(s-1)^{r-k}$$

r by s bipartite trees in which a specified light node has degree k (this also follows from formula (2.2)).

Any tree T_{n+1} for which $d_{n+1} = k$ can be constructed by partitioning the first *n* nodes into *k* non-empty subsets, forming a tree on the nodes of each subset, and then joining the (n + 1)st node to some node of each of the *k* trees. If we count the number of ways of doing these things and appeal to Theorem 3.2, we obtain the identity

(3.4)
$$\binom{n-1}{k-1} n^{n-k} = \frac{1}{k!} \sum \binom{n}{j_1, \ldots, j_k} j_1^{j_1-1} \cdots j_k^{j_k-1},$$

where the sum is over all compositions of n into k positive integers. Conversely, if identity (3.4) can be established by some other means, then Theorem 3.2 and the formula $T(n) = n^{n-2}$ follow immediately by induction. Robertson (1964) followed this approach and obtained (3.4) as a special case of a multinomial extension of Abel's identity (see also Helmer (1965)).

We now give a second proof of Theorem 3.2 that is based on an idea employed by Göbel (1963) to treat a closely related problem; the argument can easily be extended to treat a more general problem that we shall mention presently. The main step is to show that

(3.5)
$$C(n,k) = \binom{n-1}{k} \sum_{t=1}^{n-k-1} C(n-k,t)k^{t}$$

where whenever necessary we adopt the convention that an empty sum equals one.

There are $\binom{n-1}{k}$ ways to choose k nodes to join to the nth node. Temporarily discard these k nodes and construct a tree T_{n-k} on the remaining nodes in which the nth node has degree t; this can be done in C(n-k, t) ways. Now reintroduce the k discarded nodes, join each of them to the nth node, and replace each of the t edges of the type jn in T_{n-k} by an edge joining j to one of the k nodes; these replacements can be made in k^t ways. The recurrence relation for C(n, k) now follows upon summing over the possible values of t. If we assume that the formula for C(m, t)

16 Inductive Arguments

holds whenever $1 \le k \le m - 1$ and m < n, then

$$C(n,k) = \binom{n-1}{k} \sum_{t=1}^{n-k-1} \binom{n-k-2}{t-1} (n-k-1)^{n-k-t-1} k^t$$
$$= k \binom{n-1}{k} (n-1)^{n-k-2} = \binom{n-2}{k-1} (n-1)^{n-k-1}.$$

Theorem 3.2 now follows by induction on n.

3.4. The Number of k-Trees. We saw in the proof of Theorem 1.1 that a tree T_{n+1} could be defined inductively as any graph obtained by joining a new node to any node in a tree T_n . This suggests the following generalization of a tree. The graph consisting of two nodes joined by an edge is a 2-tree, and a 2-tree with n + 1 nodes is any graph obtained by joining a new node to any two nodes already joined in a 2-tree with n nodes. The 2-trees with up to five nodes and the number of ways of labelling their nodes are shown in Figure 6. A *k*-tree can be defined analogously starting with a



complete k-graph, or k nodes each of which is joined to the remaining k - 1 nodes (we remark that in many papers, especially those applying graph theory to the study of electrical networks, the term k-tree refers to a forest of k disjoint trees).

Beineke and Pippert (1969) determined the number $B_k(n)$ of k-trees with n labelled nodes by an argument we shall mention later (see also Palmer (1969)). Let $C_k(n, d)$ denote the number of k-trees with n labelled nodes in which exactly d nodes are joined to each node of a given k-tuple of nodes forming a complete subgraph; Moon (1969b) pointed out that the argument used to derive equation (3.5) can easily be extended to show that

$$C_{k}(n, d) = {\binom{n-k}{d}} \sum_{t=1}^{n-d-k} C_{k}(n-d, t)(kd)^{t}$$

It now follows by induction that if $1 \le d \le n - k$, then

$$C_k(n, d) = \binom{n-k-1}{d-1} \{k(n-k)\}^{n-d-k}$$

Consequently, there are

$$R_k(n) = \sum_{d=1}^{n-k} C_k(n, d) = \{k(n-k) + 1\}^{n-k-1}$$

k-trees in which any given k-tuple of nodes forms a complete subgraph. There are $\binom{n}{k}$ ways to select a k-tuple of nodes and each k-tree contains $\{k(n-k) + 1\}$ complete k-graphs, so it must be that

$$\binom{n}{k}R_k(n) = \{k(n-k) + 1\}B_k(n).$$

This implies Beineke and Pippert's formula,

$$B_k(n) = \binom{n}{k} \{k(n-k) + 1\}^{n-k-2}$$

Notice that when k = 1 this reduces to the formula $T(n) = n^{n-2}$. Beineke and Moon (1969) gave several other derivations of the formula for $B_2(n)$, one of which is based on Clarke's proof of Theorem 3.2.

3.5. Forests of Trees with Specified Roots. Let F(n, k) denote the number of forests with *n* labelled nodes that consist of *k* disjoint trees such that *k* specified nodes belong to distinct trees.

THEOREM 3.3. If $1 \le k \le n$, then $F(n, k) = kn^{n-k-1}$.

Göbel (1963) proved this by first showing that

$$F(n,k) = \sum_{t=1}^{n-k} {\binom{n-k}{t}} k^{t} F(n-k,t);$$

this follows upon classifying the forests according to the number t of nodes that are joined to the k specified nodes. The formula for F(n, k) now follows by induction. This argument can be extended to show that there are

$$(rl+sk-kl)r^{s-l-1}s^{r-k-1}$$

r by s bipartite forests of k + l trees in which k specified dark nodes and l specified light nodes belong to distinct trees. Szwarc and Wintgen (1965) used this type of argument to prove a result equivalent to the special case k = 0 in the course of showing there are $r^{s-1}s^{r-1}$ feasible and unfeasible bases of an r by s transportation problem; this formula has also been derived by the use of generating functions when k = l by Austin (1960) and in the general case by Moon (1967b).

We saw earlier that Theorem 3.3 could be derived by Prüfer's method. Rényi (1959b) pointed out that it is also a consequence of Theorem 3.2,

19

18 Inductive Arguments

and conversely; if we are constructing a tree T_{n+1} for which $d_{n+1} = k$, then once the k nodes joined to the (n + 1)st node are chosen the remaining edges can be chosen in F(n, k) ways and, consequently, C(n + 1, k) =

 $\binom{n}{k}F(n, k)$. Rényi (1959a) deduced the formula for F(n, k) from identity (3.4) which he established by induction using generating functions (see also Riordan (1964, 1968b)).

If f is one of the v^u functions that maps $\{1, 2, ..., u\}$ into $\{1, 2, ..., v\}$, where $u \le v$, then f may be represented by a directed graph on v labelled nodes in which an arc ij is directed from i to j if and only if f(i) = j. It is not difficult to see that each connected component of such a graph consists of a collection of rooted trees whose roots determine a directed cycle (see Figure 7) or, if u < v, a directed tree that is rooted, in effect, at one





of the nodes u + 1, u + 2, ..., v. Blakely (1964) considered a problem for such mapping functions f that is equivalent to the problem treated in Theorem 3.3. (In what follows we adopt the notation $(x)_0 = 1$ and $(x)_t = x(x-1)\cdots(x-t+1)$ for $t = 1, 2, \ldots$)

If F(t, u, v) of the functions f just described are such that exactly t nodes in the graph of f belong to cycles, then

$$v^u = \sum_{t=0}^u F(t, u, v).$$

It is not difficult to see that

$$F(t, u, v) = {\binom{u}{t}}t! F(0, u - t, v)$$

for t = 0, 1, ..., u, if we adopt the convention that F(0, 0, v) = 1; if we assume that $F(0, w, v) = (v - w)v^{w-1}$ for w < u, then

$$v^{u} = F(0, u, v) + \sum_{t=1}^{u} (u)_{t}(v - u + t)v^{u-t-1}$$

= $F(0, u, v) + \sum_{t=1}^{u} (u)_{t}v^{u-t} - \sum_{t=1}^{u} (u)_{t+1}v^{u-(t+1)}$
= $F(0, u, v) + uv^{u-1}$.

The result $F(0, u, v) = (v - u)v^{u-1}$ now follows by induction since it certainly holds when u = 1. We obtain the formula in Theorem 3.3 if we let v = n and u = n - k.

3.6. Connected Graphs with One Cycle. Consider a connected directed graph, or <u>functional digraph</u>, arising from a function f that maps $\{1, 2, ..., n\}$ into $\{1, 2, ..., n\}$; such a graph consists of a collection of rooted directed trees whose roots determine a directed cycle (J. Dénes informs me that this observation was apparently first published by Suschkewitsch (1928)). Let D(n, k) denote the number of such graphs in which the cycle has length k, where $1 \le k \le n$.

THEOREM 3.4. If $1 \le k \le n$, then $D(n, k) = (n)_k n^{n-k-1}$.

This result apparently was first proved by Rubin and Sitgreaves (1954). Katz (1955) proves it by observing that if there are n_i nodes at distance i (>0) from the cycle, then the (unique) arc issuing from each such node must be directed towards one of the n_{i-1} nodes at distance i - 1 from the cycle; if we count the number of ways of forming the cycle and choosing the nodes at different distances, we find that

$$D(n,k) = (k-1)! \sum {\binom{n}{k, n_1, \ldots, n_t}} k^{n_1} n_1^{n_2} \cdots n_{t-1}^{n_t},$$

where the sum is over all compositions $(n_1, n_2, ..., n_t)$ of M = n - k into t positive integers for t = 1, 2, ..., M (we may assume $t \ge 1$ since the theorem is obviously true when k = n). The theorem now follows from the identity

(3.6)
$$\sum \frac{k^{n_1-1}}{(n_1-1)!} \cdot \frac{n_1^{n_2-1}}{(n_2-1)!} \cdots \frac{n_{t-1}^{n_t-1}}{(n_t-1)!} (n_t)^{-1} = \frac{n^{n-k-1}}{(n-k)!}$$

where the sum is over the same compositions as before.

Katz attributes the following derivation of this identity partly to J. S. Frame. We can rewrite the right hand side of (3.6) as

$$\frac{(M+k)^{M-1}}{M!} = \frac{1}{M!} \sum_{n_1=1}^{M} {\binom{M-1}{n_1-1}} k^{n_1-1} M^{M-n_1}$$
$$= \sum_{n_1=1}^{M} \frac{k^{n_1-1}}{(n_1-1)!} \cdot \frac{(M_1+n_1)^{M_1-1}}{M_1!},$$

where $M_1 = M - n_1$. The last factor in the last summand is of the same type as the original quantity on the left and can be expanded in the same way. If we iterate this expansion, letting $M_i = M_{i-1} - n_i$ for i = 2, 3, ... until finally $M_i = 0$, we obtain the left hand side of equation (3.6). (Harary

20 Inductive Arguments

and Read (1966) drew the functional digraphs with up to six nodes that have no cycles of length one; see also Harary, Read, and Palmer (1967).)

Notice that when k = 1, the graphs counted are rooted directed trees in which the root is distinguished by the presence of a loop; consequently, $T(n) = n^{-1}D(n, 1) = n^{n-2}$.

Rényi (1959b) showed, in effect, that Theorems 3.3 and 3.4 are also equivalent; once we have formed a directed cycle on k nodes the remaining arcs can be chosen in F(n, k) ways and, consequently,

$$D(n,k) = (k-1)! \binom{n}{k} F(n,k) = (n)_k n^{n-k-1}.$$

If we ignore the directions of the arcs in these graphs, it follows that there are $\frac{1}{2}D(n, k)$ connected graphs with *n* nodes and *n* edges in which the cycle has length k when $3 \le k \le n$. Various extensions of this result are known; we shall mention these and some other problems on random mapping functions *f* later.

3.7. Trees with a Given Number of Endnodes. The proof of the next result uses properties of the Stirling numbers S(n, k) of the second kind; they may be defined (see, for example, Riordan (1958; p. 33)) by the identity

(3.7)
$$x^{n} = \sum_{k=0}^{n} S(n, k)(x)_{k}$$

for n = 0, 1, Since

 $x \cdot$

$$x^{n-1} = \sum_{k=0}^{n-1} (k + x - k)S(n - 1, k)(x)_k$$
$$= \sum_{k=0}^{n-1} kS(n - 1, k)(x)_k + \sum_{k=0}^{n-1} S(n - 1, k)(x)_{k+1}$$

it follows that S(0, 0) = 1 and

(3.8)
$$S(n,k) = kS(n-1,k) + S(n-1,k-1)$$

for k = 0, 1, ..., n for $n \ge 1$. We can now derive a formula for R(n, k), the number of trees T_n with exactly k endnodes.

THEOREM 3.5. If $2 \le k \le n$, then R(n, k) = (n!/k!)S(n - 2, n - k).

Suppose we remove one of the endnodes x from a tree T_n with k endnodes; the remaining tree T_{n-1} has k or k-1 endnodes according as the node joined with x is or is not an endnode in T_{n-1} . If we count the number of ways these alternatives can occur, we are led to the recurrence relation

$$kn^{-1}R(n,k) = (n-k)R(n-1,k-1) + kR(n-1,k),$$

for k = 2, 3, ..., n and $n \ge 3$. The result now follows by induction, using relation (3.8). Notice that

$$T(n) = \sum_{k=2}^{n} R(n,k) = \sum_{k=2}^{n} \frac{n!}{k!} S(n-2, n-k)$$
$$= \sum_{k=0}^{n-2} S(n-2, k)(n)_{k} = n^{n-2}$$

by (3.7).

Rényi (1959a) attributes the preceding derivation to V. T. Sós. Beineke and Moon (1969) used this type of argument to show that there are $M(n-3, k) \cdot (n-2)_k$ 2-trees with *n* nodes in which a given pair of nodes are joined by an edge and exactly n-2-k of the remaining nodes have degree two; the numbers M(n, k) are defined by the relation

$$(2x + 1)^n = \sum_{k=0}^n M(n, k)(x)_k$$

It follows from (3.8) that there are k! S(n, k) ways to distribute *n* different objects in *k* different places in such a way that no place remains empty (classify the distributions according as the *n*th object is or is not put by itself in one of the *k* places); Rényi (1959a) used this fact to derive Theorem 3.5 by Prüfer's method. (These arguments can be used to show that there are

$$\frac{r!}{k!} \cdot \frac{s!}{l!} S(s-1, r-k) S(r-1, s-l)$$

r by s bipartite trees with k dark endnodes and l light endnodes.) The Stirling numbers S(n, k) can be expressed as a sum involving binomial coefficients; the corresponding expression for R(n, k) can also be derived directly by the method of inclusion and exclusion if one already knows the formula $T(n) = n^{n-2}$. We shall consider the distribution of the number of endnodes in a random tree later.

3.8. Recurrence Relations for T(n). Heretofore we have derived recurrence relations for the number of trees T_n in which various parameters (in addition to the number of nodes) assumed certain values. It is also possible to derive recurrence relations for T(n) itself in various ways.

Suppose we partition $n (\geq 2)$ labelled nodes into two non-empty subsets, the first having *i* nodes and the second n - i nodes, and form a tree on each subset; if we join one of the *i* nodes of the first tree to one of the n - i nodes of the second tree we obtain a tree T_n . If we perform these operations in all possible ways we obtain each tree $T_n 2(n-1)$ times; consequently,

$$2(n-1)T(n) = \sum_{i=1}^{n-1} {n \choose i} T(i)T(n-i)i(n-i)$$

(Mullin and Stanton (1967) apply this type of argument in a somewhat more general setting.)

Dziobek (1917) and Bol (1938) both derive this recurrence relation for T(n) and they both use it to derive a relation for the generating function of the numbers T(n); we shall return to that part of their arguments later. Dziobek also says, however, that R. Rothe pointed out to him that the result $T(n) = n^{n-2}$ follows by induction from the recurrence relation and the identity

$$2(n-1)n^{n-2} = \sum_{i=1}^{n-1} \binom{n}{i} i^{i-1}(n-i)^{n-i-1}.$$

This identity follows from the second identity in Table 1; it also is the special case k = 2 of identity (3.4) which we inferred from Theorem 3.2.

Perhaps it should be pointed out that Dziobek was actually treating the problem of counting the number of sets of n-1 transpositions of n objects such that each of the n! permutations of these objects can be expressed as a product of transpositions of the set; it can be shown by induction that a set of n-1 transpositions has this property if and only if the graph on n nodes whose edges *ij* correspond to the transpositions (i, j) is a tree (see also Pólya (1937; pp. 208-209)). Dénes (1959) has shown that the number of ways of representing a cyclic permutation (1, 2, ..., n) as a product of n-1 transpositions is also equal to T(n).

Another proof of the formula $T(n) = n^{n-2}$ is based on the identity

$$n^{n-1} = \sum_{j=1}^{n} {\binom{n-1}{j-1}} j^{j-2} (n-j)^{n-j};$$

this is a special case of the first identity in Table 1. Consider one of the n^{n-1} functions f mapping 1, 2, ..., n-1 into 1, 2, ..., n. We have already seen how such a function can be represented by a directed graph on n nodes. If we classify these functions according to the number of nodes in the connected component of their graph that contains the nth node we obtain the relation

$$n^{n-1} = \sum_{j=1}^{n} \binom{n-1}{j-1} T(j)(n-j)^{n-j}$$

The formula for T(n) now follows by induction.

The last derivation we give of this type is based on the fact that

(3.9)
$$\sum_{j=0}^{n-1} (-1)^j {n \choose j} (n-j)^k = 0$$

for any positive integer k less than n. The left member is the number of ways, using the method of inclusion and exclusion, of distributing k different objects in n different places in such a way that no place remains empty; it also is equal to $\Delta^n 0^k = n! S(k, n)$.

Moon (1963) observed that if there are C(n, m) connected graphs with n labelled nodes and m edges and H(n, m, l) of these have exactly l end-nodes, then

$$H(n, m, l) = \sum_{j=l}^{n-1} (-1)^{j-l} {j \choose l} {n \choose j} C(n-j, m-j)(n-j)^{j},$$

if $n \ge 3$ (Gilbert (1956) gave a generating function for the numbers C(n, m)). This follows from the method of inclusion and exclusion and the fact that two endnodes of a connected graph cannot be joined to each other if $n \ge 3$. If m = n - 1, then these graphs are trees and H(n, n - 1, 0) = 0, by Lemma 1.1. Therefore,

(3.10)
$$\sum_{j=0}^{n-1} (-1)^j \binom{n}{j} T(n-j)(n-j)^j = 0$$

and the formula for T(n) now follows by induction using the case k = n - 2 of the identity (we shall describe later another derivation due to Dziobek (1917) of a relation very similar to this one). Notice that this yields another proof of Theorem 3.5, since

$$R(n,k) = H(n,n-1,k) = \sum_{j=k}^{n-1} (-1)^{j-k} {j \choose k} {n \choose j} (n-j)^{n-2}$$

= ${n \choose k} \sum_{h=0}^{n-k} (-1)^{h} {n-k \choose h} \{(n-k)-j\}^{n-2} = \frac{n!}{k!} S(n-2,n-k).$

3.9. Connected Graphs with Unlabelled Endnodes. Moon (1969a) also used the formula for H(n, m, l) to obtain a formula for the number E(n + k, m + k, k) of connected graphs G with n + k nodes and m + k edges such that $n (\geq 3)$ of the nodes are labelled and are not endnodes and k of the nodes are not labelled and are endnodes. If we remove the k endnodes of such a graph G, then the remaining graph G' is one of the H(n, m, l) connected graphs with m edges and n labelled nodes of which l are endnodes, for some integer l not exceeding k.

2+c.l.t.

24 Inductive Arguments

The number of ways of joining k unlabelled nodes to such a graph G' so that these k nodes are the only endnodes in the resulting graph G is equal to the coefficient of x^k in

 $(x + x^{2} + \cdots)^{l}(1 + x + x^{2} + \cdots)^{n-l} = x^{l}(1 - x)^{-n}$

or

$$(-1)^{k-l}\binom{-n}{k-l} = \binom{k+n-1-l}{n-1}.$$

Therefore,

$$E(n + k, m + k, k)$$

$$= \sum_{l=0}^{k} (-1)^{k-l} {\binom{-n}{k-l}} H(n, m, l)$$

$$= \sum_{j=0}^{n-1} (-1)^{j+k} {\binom{n}{j}} C(n-j, m-j)(n-j)^{j} \sum_{l=0}^{j} {\binom{-n}{k-l}} {\binom{j}{l}}$$

$$= \sum_{j=0}^{n-1} (-1)^{j} {\binom{n}{j}} {\binom{k+n-1-j}{k}} C(n-j, m-j)(n-j)^{j}.$$

If we wish to count the number $T^*(n)$ of trees with $n \ (\geq 3)$ nodes in which all nodes except endnodes are labelled, we replace n + k by n and C(n - j, m - j) by $(n - k - j)^{n-k-j-2}$, and sum from k = 2 to k = n - 1; hence,

$$T^{*}(n) = \sum_{k=2}^{n-1} \sum_{j=0}^{n-k-1} (-1)^{j} \binom{n-k}{j} \binom{n-1-j}{k} (n-k-j)^{n-k-2}.$$

The last formula is equivalent to a result obtained earlier by Harary, Mowshowitz, and Riordan (1969).

APPLICATIONS OF

GENERATING FUNCTIONS

4

4.1. Counting Connected Graphs. Generating functions provide a useful tool for the solution of many combinatorial problems. We now illustrate their application to certain enumeration problems for labelled trees; we shall give more examples later when we consider the distribution of various parameters associated with trees.

Let g_n denote the number of graphs G_n each component of which enjoys a certain property P and let c_n denote the number of these that are connected. It is not difficult to see that there are

$$\frac{1}{2}\sum_{k=1}^{n-1} \binom{n}{k} c_k c_{n-k} = \frac{1}{2}n! \sum_{k=1}^{n-1} \frac{c_k}{k!} \cdot \frac{c_{n-k}}{(n-k)!}$$

of these graphs G_n with exactly two connected components. Thus if

$$C = C(x) = \sum_{n=1}^{\infty} c_n \frac{x^n}{n!}$$

is the (exponential) generating functions for the connected graphs with property P, then the coefficient of $x^n/n!$ in $\frac{1}{2}C^2(x)$ is the number of 2component graphs G_n with property P. More generally, the generating function for the k-component graphs with property P is $C^k(x)/k!$. Hence, if

$$G = G(x) = \sum_{n=1}^{\infty} g_n \frac{x^n}{n!}$$

25

is the generating function for all graphs G_n with property P, then

$$G = C + \frac{1}{2!}C^2 + \frac{1}{3!}C^3 + \cdots = e^C - 1.$$

This relation appears in many papers (see, for example, Riddell and Uhlenbeck (1953) and Gilbert (1956)); the argument can easily be modified to cover situations where more parameters are involved or where the nodes are not labelled. Another derivation is based on the fact that the derivative of a generating function for labelled graphs, multiplied by x, gives the generating function for the corresponding rooted graphs; since the root node of a graph effectively singles out one connected component of the graph, it follows that xG' = xC'(1 + G) which implies that $C = \ln (1 + G)$ or $G = e^{C} - 1$.

4.2. Counting Rooted Trees and Forests. We now specialize the preceding argument to trees. If

$$Y = Y(x) = \sum_{n=1}^{\infty} nT(n) \frac{x^n}{n!}$$

denotes the generating function for rooted trees, then $(1/k!)Y^k$ is the generating function for forests of k rooted trees. If we join each root node of a forest of rooted trees to a new node we obtain, in effect, a rooted tree with one more node than the original forest. Every rooted tree (or at least those with more than one node) can be obtained uniquely this way. It follows, therefore, that Y satisfies the functional relation

 $Y = x + xY + \frac{xY^2}{2!} + \cdots = xe^{y},$

or

$$(4.1) x = Ye^{-y}$$

This argument is due to Pólya (1937) who uses Lagrange's inversion formula to deduce from (4.1) that

$$Y=\sum_{n=1}^{\infty}n^{n-1}\frac{x^n}{n!}$$

from which it follows that $T(n) = n^{n-2}$.

Lagrange's formula (see, for example, Whittaker and Watson (1946)) states that if $z = x\phi(z)$,

then

$$f(z) = f(0) + \sum_{n=1}^{\infty} \frac{x^n}{n!} D^{n-1} [f'(z)\phi^n(z)]_{z=0},$$

subject to certain conditions on the functions ϕ and f. If z = Y, $\phi(z) = e^{Y}$, and $f(Y) = Y^{k}$, then

$$D^{n-1}[f'(Y)\phi^{n}(Y)]_{Y=0} = D^{n-1}[k Y^{k-1}e^{nY}]_{Y=0}$$

= $k \sum_{i=0}^{n-1} {n-1 \choose i} D^{i}(Y^{k-1}) D^{n-1-i}(e^{nY})\Big|_{Y=0}$
= $k {n-1 \choose k-1} (k-1)! n^{n-k} = k n^{n-k-1}(n)_{k}.$

Therefore, if $Y = xe^{Y}$, where Y(0) = 0, then

(4.2)
$$\frac{Y^k}{k!} = \sum_{n=k}^{\infty} \binom{n}{k} k n^{n-k-1} \frac{x^n}{n!}$$

for k = 1, 2, ...

Notice that formula (4.2) is equivalent to identity (3.4) which we derived by a combinatorial argument. It follows from (4.2) that there are $\binom{n}{k}kn^{n-k-1}$ forests with *n* labelled nodes consisting of *k* rooted trees, for $1 \le k \le n$; this result is equivalent to Theorem 3.3 since the *k* root nodes can be selected in $\binom{n}{k}$ ways. As a partial check notice that the total number of forests of rooted trees on *n* nodes is equal to

$$\sum_{k=1}^{n} \binom{n}{k} k n^{n-k-1} = (n+1)^{n-1}$$

as it should be, since there is a one-to-one correspondence between forests of rooted trees with *n* nodes and trees with n + 1 nodes rooted at the (n + 1)st node. (Riordan (1968b) has pointed out that there are $\binom{n}{k}k^{n-k}$ forests (of *n* labelled nodes) of *k* rooted trees in which every non-root node is joined directly to a root node and that there are $\frac{n!}{k!}\binom{n-1}{k-1}$ forests of *k* paths each rooted at an endnode.)

4.3. Counting Unrooted Trees and Forests. Dziobek (1917) and Bol (1938) both deduce relation (4.1) from the recurrence relation

(4.3)
$$2(n-1)T(n) = \sum_{i=1}^{n-1} {n \choose i} T(i)T(n-i)i(n-i)$$

which we derived in Section 3.8. Let

$$y = y(x) = \sum_{n=1}^{\infty} T(n) \frac{x^n}{n!}$$

denote the generating function for (unrooted) labelled trees so that

If we multiply both sides of the above recurrence relation by $x^n/n!$ and sum over *n*, we obtain the relation $2Y - 2y = Y^2$, or

xv'.

$$(4.5) y = Y - \frac{1}{2}Y^2.$$

It follows from (4.4) and (4.5) that

$$\frac{dx}{x} = \frac{1 - Y}{Y} \, dY$$

and this implies that $x = Ye^{-Y}$, as required (the constant of integration must be zero since T(1) = 1).

Bol, having established equation (4.1), uses Cauchy's integral formula to determine the coefficients in Y. Dziobek makes the substitution

$$x^{j} = Y^{j}e^{-jY} = Y^{j} + (-j)Y^{j+1} + \frac{j^{2}Y^{j+2}}{2!} + \cdots + \frac{(-j)^{n-j}Y^{n}}{(n-j)!} + \cdots$$

in the right hand side of

$$Y = T(1)x + 2 \cdot T(2) \frac{x^2}{2!} + \cdots + j \cdot T(j) \frac{x^j}{j!} + \cdots,$$

for j = 1, 2, ..., and equates the coefficients of Y^n in the resulting expression; this yields (after multiplying through by n!) the relation

$$\sum_{j=0}^{n-1} (-1)^{j} {\binom{n}{j}} T(n-j)(n-j)^{j+1} = 0$$

for n = 2, 3, ... (cf. equation (3.10)). The result $T(n) = n^{n-2}$ now follows by induction using identity (3.9).

Rényi (1959a) used relations (4.2) and (4.5) to derive a formula for the number $f_k(n)$ of forests with n labelled nodes consisting of k (unrooted) trees.

THEOREM 4.1. If $1 \le k \le n$, then

$$f_k(n) = \binom{n}{k} n^{n-k-1} \sum_{i=0}^k \left(-\frac{1}{2}\right)^i \binom{k}{i} (k+i) \frac{(n-k)_i}{n^i}$$

The generating function for forests of k trees is $y^k/k!$, by the argument

given in Section 4.1; it follows, therefore, from (4.5) that

$$\sum_{n=k}^{\infty} f_k(n) \frac{x^n}{n!} = \frac{1}{k!} y^k = \frac{1}{k!} (Y - \frac{1}{2} Y^2)^k$$
$$= \frac{1}{k!} \sum_{i=0}^k \binom{k}{i} (-\frac{1}{2})^i Y^{k+i}.$$

If we use formula (4.2) to determine the coefficient of x^n in the right hand member, we obtain the required formula for $f_k(n)$. A few special cases of this formula are

$$f_{1}(n) = n^{n-2}, \quad f_{2}(n) = \frac{1}{2}n^{n-4}(n-1)(n+6),$$

$$f_{3}(n) = \frac{1}{8}n^{n-6}(n-1)(n-2)(n^{2}+13n+60), \dots,$$

$$f_{n-3} = \frac{1}{2}\binom{n}{4}(n^{2}+3n+4),$$

$$f_{n-2}(n) = 3\binom{n+1}{4}, \quad f_{n-1}(n) = \binom{n}{2}, \text{ and } f_{n}(n) = 1$$

If we let c(k, h) denote the coefficient of n^{n-h} in the formula for $f_k(n)$, for h = 1, 2, ..., 2k, we find after some simplification that

$$c(k, 1) = \frac{1}{k!} \sum_{i=0}^{k} (-\frac{1}{2})^{i} \binom{k}{i} (k+i) = 0$$

and

$$c(k,2) = \frac{-1}{k!} \sum_{i=0}^{k} \left(-\frac{1}{2}\right)^{i} (k+i) \binom{k}{i} \binom{k+i}{2} = \frac{\left(\frac{1}{2}\right)^{k-1}}{(k-1)!}$$

Therefore,

 f_n

$$\lim_{n\to\infty}\frac{f_k(n)}{n^{n-2}}=\frac{(\frac{1}{2})^{k-1}}{(k-1)!},$$

for each fixed k; if F(n) denotes the total number of forests with n labelled nodes then it follows from Tannery's theorem (see Bromwich (1931)) that

$$\lim_{n\to\infty}\frac{F(n)}{n^{n-2}}=\sum_{k=1}^{\infty}\frac{(\frac{1}{2})^{k-1}}{(k-1)!}=e^{1/2}.$$

(We would expect, therefore, that the average number of trees in a random forest with a large number of nodes would be about $\frac{3}{2}$.) Rényi shows that

$$F(n) = \sum_{k=1}^{n} H_{k}(-1)kn^{n-k-1}(n)_{k}$$

where

$$H_k(x) = \frac{1}{k!} e^{x^2/2} \frac{d^k}{dx^k} \left(e^{-x^2/2} \right)$$

is the kth Hermite polynomial. Dénes (1959) pointed out that $f_k(n)$ is also given by the formula

$$f_k(n) = n! \sum \prod_{j=1}^n \frac{1}{a_j!} \left(\frac{j^{j-2}}{j!}\right)^{a_j}$$

where the sum is over all non-negative integer solutions of the equations

$$\sum_{j=1}^n a_j = k \quad \text{and} \quad \sum_{j=1}^n j a_j = n.$$

Riordan (1964) derived a pair of inverse relations that involve the numbers $f_k(n)$. In (1968b) he showed that there are

$$\frac{n!}{2^{k}k!}\sum_{j=0}^{k} \binom{k}{j}\binom{n-j-1}{k-j-1}$$

forests with n labelled nodes that consist of k paths. He also derived recurrences and congruences involving these and related numbers.

4.4. Bipartite Trees and Forests. Austin (1960) and Scoins (1962) derived the formula for T(r, s), the number of r by s bipartite trees, by a slight modification of Pólya's argument. If

 $R = R(x, y) = \sum_{r,s} rT(r, s) \frac{x^r}{r!} \cdot \frac{y^s}{s!}$

and

$$S = S(x, y) = \sum_{r,s} sT(r, s) \frac{x^r}{r!} \cdot \frac{y^s}{s!}$$

denote the generating functions for bipartite trees rooted at a dark node and a light node, then essentially the same argument we used before shows that $R = xe^s$ and $S = ye^R$. Consequently,

$$R = x \exp y \exp R$$
,

and we can apply Lagrange's formula with z = R, $\phi(R) = \exp y \exp R$, and $f(R) = R^k$. If we expand $\phi^r(R)$ as a power series in R we find that

$$D^{r-1}[f'(R)\phi^r(R)]_{R=0} = D^{r-1}[kR \exp ry \exp R]_{R=0}$$
$$= k(r-1)_{k-1} \sum_{s=0}^{\infty} \frac{(ry)^s s^{r-k}}{s!}.$$

Hence,

$$R^{k} = \sum_{r,s} k(r)_{k} r^{s-1} s^{r-k} \frac{x^{r}}{r!} \cdot \frac{y^{s}}{s!};$$

in particular,

$$R = \sum_{r,s} r^s s^{r-1} \frac{x^r}{r!} \cdot \frac{y^s}{s!},$$

which implies that $T(r, s) = r^{s-1}s^{r-1}$.

More generally, it can be shown that

(4.6)
$$R^{k}S^{l} = \sum_{r,s} (rl + sk - kl)(r)_{k}(s)_{l}r^{s-l-1}S^{r-k-1}\frac{x^{r}}{r!} \cdot \frac{y^{s}}{s!};$$

this can be established by using Lagrange's formula with $f(R) = R^k y^l e^{lR}$ or by substituting the series for R^j in the power series expansion of $R^k S^l = R^k y^l e^{lR}$, for j = k, k + 1, ... and then simplifying (see Austin (1960) and Moon (1967b)). It follows, therefore, that there are

(4.7)
$$\binom{r}{k}\binom{s}{l}(rl+sk-kl)r^{s-l-1}s^{r-k-1}$$

r by s bipartite forests of k + l trees k of which are rooted at a dark node and l at a light node; this is equivalent to the bipartite analogue of Theorem 3.3 stated earlier.

The number $f_k(r, s)$ of r by s bipartite forests of k (unrooted) trees can be determined by the same method as was used to prove Theorem 4.1. Let

$$B = B(x, y) = \sum_{r,s} T(r, s) \frac{x^r}{r!} \cdot \frac{y^s}{s!}$$

denote the generating function for (unrooted) bipartite trees; notice that

$$x \frac{\partial B}{\partial x} = R$$
 and $y \frac{\partial B}{\partial y} = S$

The relation

$$B = R + S - RS$$

can be established by verifying that both sides have the same derivatives and vanish when x = y = 0 or by considering a bipartite analogue of the recurrence formula (4.3). It follows, therefore, that

$$\sum_{r,s} f_k(r,s) \frac{x^r}{r!} \cdot \frac{y^s}{s!} = \frac{1}{k!} B^k = \frac{1}{k!} (R + S - RS)^k$$
$$= \sum_{h=0}^k \frac{(-1)^h}{h!} \sum_{a+b=k-h} \frac{R^{h+a}}{a!} \cdot \frac{S^{h+b}}{b!}$$

2*

If we use equation (4.6) to determine the coefficient of $x^r y^s$ in the last expression, we obtain the formula

$$f_{k}(r,s) = r^{s-1}s^{r-1} \sum_{h=0}^{k} \frac{(-1)^{h}}{h!} \frac{(r)_{h}}{r^{h}} \frac{(s)_{h}}{s^{h}}$$

$$\times \sum_{a+b=k-h} \{r(h+b) + s(h+a) - (h+a)(h+b)\}$$

$$\times \binom{r-h}{a}\binom{s-h}{b}r^{-b}s^{-a},$$

if $r + s \ge k$; in particular, $f_1(r, s) = r^{s-1}s^{r-1}$ and

$$f_2(r,s) = r^{s-2}s^{r-2}(r^2 + s^2 - rs + r + s - 2).$$

4.5. Counting Trees by Number of Inversions. Suppose the tree T_n is rooted at node n; if g(i) denotes the number of nodes j such that j > i and the (unique) path in T_n from j to n passes through i, then $\sum_{i=1}^{n-1} g(i)$ is the number of *inversions* of T_n (the number of inversions of a permutation is the number of transpositions needed to restore the natural order). Mallows and Riordan (1968) derived a functional relation for the polynomials $J_n(x)$ in which the coefficient of x^t is the number of trees T_n with t inversions,

for
$$t = 0, 1, \dots, \binom{n-1}{2}$$
.

Let $K_n(x)$ denote the corresponding polynomial for *planted* trees T_n , that is, rooted trees in which the root is an endnode. If the root *n* is joined only to node *j* then T_n has (n - 1) - j more inversions than the tree T_{n-1} obtained from T_n by removing *j* and joining *n* directly to the nodes originally joined to *j* (we should also diminish by one the labels of all nodes *y* such that y > j, but this does not affect the number of inversions). It follows, therefore, that

$$K_n(x) = (1 + x + \cdots + x^{n-2})J_{n-1}(x)$$

for n = 2, 3,

Any rooted tree can be formed by identifying the roots of a forest of planted subtrees. If the tree T_{n+1} is rooted at node n + 1 let T^* denote the planted subtree that contains, say, the 1st node; if T^* contains k nodes besides the 1st and (n + 1)st nodes, then there are $\binom{n-1}{k}$ choices possible for these nodes. The number of inversions of T_{n+1} equals the number of inversions of the rooted subtrees determined by the root n + 1 and the nodes not in T^* . Hence,

(4.8)
$$J_{n+1}(x) = \sum_{k=0}^{n-1} {\binom{n-1}{k}} K_{k+2}(x) J_{n-k}(x)$$

for n = 1, 2, ..., since the number of inversions of a tree depends only on the relative sizes of the labels of the nodes. If

 $J = J(x, y) = \sum_{n=1}^{\infty} J_{n+1}(x) \frac{y^n}{n!}$

and

$$K = K(x, y) = \sum_{n=1}^{\infty} K_{n+1}(x) \frac{y^n}{n!}$$

then it follows from (4.7) that

$$\frac{\partial J}{\partial y} = \frac{\partial K}{\partial y} J;$$

this implies that

$$(4.9) J = e^{\kappa}$$

or

$$\sum_{n=0}^{\infty} J_{n+1}(x) \frac{y^n}{n!} = \exp \sum_{n=1}^{\infty} J_n(x) \frac{x^n - 1}{x - 1} \cdot \frac{y^n}{n!}$$

(The constant of integration is determined by the fact that J = 1 and K = 0 when y = 0.)

Mallows and Riordan derived relation (4.9) first (by an argument similar to the argument used to establish relation (4.1)) and then deduced (4.8) as a consequence; they show that the polynomials $J_n(x)$ appear in the generating function of the cumulants of the lognormal distribution. The first few values of $J_n = J_n(x)$ are found to be

and

$$J_5 = 24 + 36x + 30x^2 + 20x^3 + 10x^4 + 4x^5 + x^6.$$

 $J_1 = J_2 = 1$, $J_3 = 2 + x$, $J_4 = 6 + 6x + 3x^2 + x^3$.

4.6. Connected Graphs with Given Blocks. Uhlenbeck and Ford (1962, 1963) discuss certain problems in physics that lead to enumeration problems for graphs (the number of terms in the *n*th successive approximation to certain functions equals the number of graphs with certain properties; see also, for example, Temperley (1958, 1964) and Groeneveld (1967a,b)). Before proving one of their earlier results we introduce some more terminology.

The automorphism group of a graph is the set of all permutations α of the nodes such that nodes x and y are joined by an edge if and only if nodes $\alpha(x)$ and $\alpha(y)$ are joined. The group of the complete k-graph, for example,

is the symmetric group of order k! and the group of a k-cycle is the dihedral group of order 2k. If the group of a graph G with n nodes has order g, then there are n!/g different labellings of the nodes of G; we shall use later the equivalent result that there are n!/g ways to construct a graph isomorphic to G on a given set of n labelled nodes. This follows from the result that if A is a group of permutations acting on an object set X, then the index of the stabilizer of an object x in X equals the number of objects in the orbit of x.

A cut-node of a graph is a node whose removal increases the number of connected components in the graph; a block of a graph is a maximal connected subgraph that contains no cut-nodes of itself. (Notice that a single node is not a block unless it forms a connected component by itself.) A non-trivial tree can be defined as a connected graph all of whose blocks are complete 2-graphs (that is, single edges joining two nodes). Any connected graph can be thought of as a tree-like structure consisting of a collection of blocks attached to each other at cut-nodes. For example, the connected graphs whose blocks consist of one complete 2-graph and two complete 3-graphs and the number of ways of labelling their nodes are shown in Figure 8.



FIGURE 8

Let B_i denote some block with m_i (>1) nodes whose automorphism group has order g_i , for i = 1, 2, ..., b. Ford and Uhlenbeck (1956a) extended Pólya's argument to determine the number $T(n; c_1, c_2, ..., c_b)$ of rooted connected graphs G with n labelled nodes c_i of whose blocks are isomorphic to B_i , for i = 1, 2, ..., b.

THEOREM 4.2. If

$$\sum_{i=1}^{b} c_i(m_i - 1) = n - 1,$$

then

$$T(n; c_1, c_2, \ldots, c_b) = \frac{(n-1)! n^{2c_i}}{\Pi(g_i/m_i)^{c_i} c_i!}$$

The c's and the m's must satisfy the first equation if the total number of nodes in G is to be n. Let us first consider the case b = 1 when there is only

one type of block available. If

$$U(x) - x = \sum_{n=m}^{\infty} T(n; c) \frac{x^n}{n!}$$

denotes the generating function for the number of rooted connected graphs whose blocks are isomorphic to $B = B_1$ (notice that T(n, c) = 0 unless n = c(m - 1) + 1, where $m = m_1$), then

$$(4.10) U = U(x) = x + U_1(x) + U_2(x) + \cdots$$

where $U_j(x)$ is the generating function for those graphs in which the root belongs to exactly *j* copies of *B*. We first determine a relation for $U_1(x)$.

Consider a graph H with n labelled nodes that consists of m rooted connected components; each block is isomorphic to B except that one component is singled out and consists of an isolated node r and some of the other components may also consist of an isolated node. The number of such graphs H (that are, in effect, doubly rooted at an isolated node r) is equal to the coefficient of $x^n/n!$ in $xU^{m-1}(x)/(m-1)!$. The factor x takes into account the isolated root node r, and the (m-1)! is present because there is no significance to the ordering of the remaining components (the fact that some of these other components may also consist of an isolated node is why we defined U(x) to contain the term x).

There are m!/g ways to join the roots of the components of such a graph H so that the subgraph determined by these nodes is isomorphic to B, where $g = g_1$ denotes the order of the group of B. The resulting graph is connected, each of its blocks is isomorphic to B, and the root node r belongs to just one copy of B. It follows, therefore, that the generating function for the number of such graphs satisfies the relation

(4.11)
$$U_1(x) = x \frac{m}{g} U^{m-1}(x)$$

Graphs G in which the root belongs to j copies of B may be constructed by identifying the roots of j graphs in which the root belongs to just one copy of B. Consequently,

(4.12)
$$U_j(x) = \frac{x}{j!} \left(\frac{U_1(x)}{x} \right)^j,$$

for j = 1, 2, ...; the x's take into account the nodes that are lost in this process and the j! reflects the fact that there is no significance to the ordering of the j graphs.

When we combine equations (4.10)-(4.12) we obtain the relation

$$U=x\exp\frac{m}{g}\ U^{m-1}.$$

If we apply Lagrange's formula with z = U, $\phi(U) = \exp \frac{m}{g} U^{m-1}$, and f(U) = U, we find that if c(m-1) = n - 1, then

$$T(n, c) = D^{n-1}[f'(U)\phi^n(U)]_{U=0} = D^{n-1}\left[\sum_{j=0}^{\infty} \left(\frac{mn}{g} U^{m-1}\right)^j / j!\right]_{U=0}$$
$$= \frac{(n-1)! n^c}{(g/m)^c c!}.$$

Notice that if B is the complete 2-graph (so that g = m = 2 and c = n - 1) then the formula reduces to n^{n-1} , the number of rooted trees with n labelled nodes.

In the general case, when there are an arbitrary number b of blocks available, let

$$U(x; y_1, \ldots, y_b) - x = \sum_n \left\{ \sum T(n; c_1, \ldots, c_b) y_1^{c_1} \cdots y_b^{c_b} \right\}_{n!}^{x^n}$$

denote the generating function for the number of rooted connected graphs that can be formed using the blocks B_i ; the outer sum starts at $n = \min \{m_1, m_2, \ldots, m_b\}$ and the inner sum is over all admissible values of the c_i 's. The relation

$$U = x \exp\left\{\sum_{i=1}^{b} \frac{m_i}{g_i} y_i U^{m_i - 1}\right\}$$

can be established by the same argument as before except that now, in determining U_1 , we must take into account that the root can belong to any one of the blocks B_i ; the y_i identifies the type of block to which the root belongs. The theorem now follows upon applying Lagrange's formula to this relation. (Notice that if we want to count unrooted connected graphs formed from the blocks B_i , then we should decrease the exponent of n by one.)

COROLLARY 4.2.1. If $\sum_{i=3}^{b} c_i(i-1) = n-1$, then there are

$$\frac{1}{2} \frac{(n-1)!}{\prod c_i!} (\frac{1}{2}n)^{\sum c_i-1}$$

connected graphs with n labelled nodes among whose blocks are c_i cycles of length i, for $3 \le i \le b$.

COROLLARY 4.2.2. If
$$\sum_{i=2}^{b} c_i(i-1) = n-1$$
, then there are

~

$$\frac{(n-1)! n^{\sum c_i-1}}{\prod\{(i-1)!\}^{c_i} c_i!}$$

connected graphs with n labelled nodes among whose blocks are c_i complete *i*-graphs, for $2 \le i \le b$.

Husimi (1950) derived Corollary 4.2.2 by an extension of Bol's argument; Ford and Uhlenbeck (1956a) showed that Bol's method could also be used to prove Theorem 4.2. Notice that Theorem 4.2 contains Theorem 3.4. in effect, as a special case.

If b = n and we sum the formula in Corollary 4.2.2 over all solutions in non-negative integers to the equations

$$\sum_{i=2}^{n} c_{i}(i-1) = n-1 \quad \text{and} \quad \sum_{i=2}^{n} c_{i} = k,$$

we find that there are $S(n - 1, k)n^{k-1}$ connected graphs with *n* labelled nodes and *k* blocks each of which is a complete graph, where S(n - 1, k)denotes a Stirling number of the second kind and $1 \le k \le n - 1$ (notice that $S(n - 1, k)n^{k-1} = n^{n-2}$ when k = n - 1); this result is given by Kreweras (1970).

He proves Corollary 4.2.2 by associating a bipartite tree T = T(G) with every connected graph G; the dark nodes, say, of T correspond to the nodes of G, the light nodes correspond to the blocks of G, and a dark node p is joined to a light node q if and only if in G the node corresponding to p belongs to the block corresponding to q (a bipartite tree T can be associated with some graph G in this manner if and only if all the endnodes of T are dark). Thus the number of connected graphs with n labelled nodes and $\sum_{i=2}^{b} c_i = k$ blocks of which c_i are complete *i*-graphs is equal to the number of n by k bipartite trees in which c_i light nodes have degree *i*, for $2 \le i \le b$; the formula in Corollary 4.2.2 now follows from the formula (2.2) for the number of bipartite trees with given degree sequences. Theorem 4.2 can also be proved in essentially the same way.

Ford and Uhlenbeck, in (1956b) and (1957), investigated the asymptotic behaviour of the number of graphs with certain properties. They showed, in particular, that the number of connected graphs with n labelled nodes each of whose blocks is a cycle or a complete 2-graph is asymptotically equal to

$$n! \frac{b}{2\sqrt{\pi}} \alpha^{-n+(1/2)} n^{-(5/2)}$$

where $b \doteq 0.87170$ and $\alpha \doteq 0.23874$, as *n* tends to infinity. They also considered the distribution of the nodes among the different blocks in a connected graph formed from a given collection of blocks.

Good (1965) has developed a multivariate generalization of Lagrange's theorem that he applies to various enumeration problems for different

types of trees; his method is particularly well adapted for problems involving constraints on the colouring and ordering of the nodes with different constraints, perhaps, for nodes at different distances (generations) from a root node. Knuth (1968b) points out that one of Good's results provides another proof of Theorem 2.2.

THE MATRIX TREE THEOREM

5

5.1. Introduction. Many papers have been written in which certain concepts of graph theory are applied to the study of electrical networks. The following quotation is taken from a book by Seshu and Reed (1961; p. 24).

"The 'tree' is perhaps the single most important concept in graph theory insofar as electrical network theory is concerned.... The number of independent Kirchhoff equations, the method of choosing independent equations, the structure of the coefficient matrices, and the topological formulas for network functions, are all stated in terms of the single concept of a tree."

Our main object in this chapter is to derive a result that expresses the number of spanning trees of a graph as the determinant of a matrix whose entries depend on the graph. (The determinant arises in applying Cramer's rule to solve certain sets of equations associated with an electrical network; for additional material on the application of graph theory to electrical networks see, for example, Weinberg (1962), Bryant (1967), or Slepian (1968).)

5.2. The Incidence Matrix of a Graph. Let G denote a graph with $n (\geq 2)$ labelled nodes and b edges; suppose we number the edges of G from 1 to b and orient each edge arbitrarily (we ignore the orientations of the edges when considering subgraphs of G). The (node-edge or node-branch) *incidence matrix* of G is the n by b matrix $A_a = [a_{ij}]$ in which a_{ij} equals +1 or -1 if the *j*th edge is oriented away from or towards the *i*th node and zero otherwise. (An example of a graph and its incidence matrix is given in Figure 9.)





Notice that each column of an incidence matrix A_a contains one +1, one -1, and n - 2 zeros. The following result is essentially due to Kirchhoff (1847).

LEMMA 5.1. If the graph G has n nodes and is connected, then the rank of its incidence matrix A_a is n - 1.

The sum of any r rows of A_a must contain at least one non-zero entry if r < n for G would not be connected otherwise; this implies that no r rows are linearly dependent if r < n. The result now follows from the fact that the sum of all n rows vanishes. (If G has s connected components then the rank of A_a is n - s; this follows upon applying this lemma to the submatrices corresponding to the connected components of G.)

The reduced incidence matrix A of a connected graph G is the matrix obtained from the incidence matrix A_a by deleting some row, say the *n*th. (If G has s components, then A is obtained by removing s rows from A_a corresponding to nodes in different components.) The matrix A has the same rank and furnishes the same information as A_a .

The next result was proved by Poincaré (1901).

LEMMA 5.2. If B is any non-singular square submatrix of A_a (or A), then the determinant of B is ± 1 .

If B is non-singular then each column of B must contain at least one non-zero entry but not all columns can contain two non-zero entries; hence, some column of B must contain just one non-zero entry. The required result now follows by induction if we expand the determinant of B along this column.

The next result was proved by Chuard (1922).

LEMMA 5.3. If B is a submatrix of order n - 1 of A, then B is nonsingular if and only if the edges corresponding to the columns of B determine a spanning subtree of G.

If H denotes the spanning subgraph of G whose n - 1 edges correspond to the columns of B, then B is the reduced incidence matrix of H. Hence, B is non-singular \Leftrightarrow rank (B) = $n - 1 \Leftrightarrow H$ is connected $\Leftrightarrow H$ is a tree, by Lemmas 5.1 and 1.2.

5.3. The Matrix Tree Theorem. Several people have proved the following theorem or results closely related to it; see, for example, Brooks, Smith, Stone, and Tutte (1940), Lantieri (1950), Okada and Onodera (1952), Trent (1954), Uhlenbeck and Ford (1962), Dambit (1965), Hutschenreuther (1967), and Rényi (1970).

THEOREM 5.1. If A is a reduced incidence matrix of the graph G, then the number of spanning trees of G equals the determinant of $A \cdot A^{tr}$.

The Binet-Cauchy theorem states that if R and S are matrices of size p by q and q by p where $p \le q$, then

$$\det(RS) = \sum \det(B) \cdot \det(C),$$

where the sum is over the square submatrices B and C of R and S of order p such that the columns of R in B are numbered the same as the rows of S in C. If we apply this to A and A^{tr} , assuming that $n - 1 \le b$, and appeal to Lemma 5.2, we find that

$$\det (A \cdot A^{tr}) = \sum \det (B) \cdot \det (B^{tr}) = \sum {\det (B)}^2 = \sum 1,$$

where the last sum is over all non-singular (n - 1) by (n - 1) submatrices of A. The required result now follows from Lemma 5.3.

If e_1, e_2, \ldots, e_b are variables identified with the edges of the (connected) graph G, let $M(e) = [m_{ij}]$ denote the n by n matrix in which m_{ij} equals $-e_k$ if edge e_k joins the distinct nodes i and j and zero otherwise, and m_{ii} equals the sum of the edges incident with node i; let $M_i(e)$ denote the cofactor of m_{ii} in M(e). A tree product is a product $\Pi(T)$ of edges of a spanning subtree T of G.

THEOREM 5.2. If $n \ge 2$, then

$$M_n(e) = \sum \Pi(T),$$

where the sum is over all spanning subtrees T of G.

COROLLARY 5.2.1. If c(G) denotes the number of spanning trees of G and M denotes the matrix obtained from M(e) by replacing each e_i by 1, then $c(G) = M_n$.

It is easy to verify that $M_n(e) = \det(AYA^{tr})$, where $Y = [y_{ij}]$ is the b by b diagonal matrix such that $y_{ii} = e_i$. The result now follows by applying the Binet-Cauchy theorem to the product AYA^{tr} . (If the row and column sums of a matrix all vanish, as they do for M(e), then the cofactors of its

entries are all equal; hence, the sum of the tree products equals the cofactor of any entry of the matrix M(e).)

The sum of the tree products of the spanning trees of a graph G is sometimes called the *tree polynomial* of G. If G is the graph in Figure 9, for example, we find that

$$M_4(e) = \begin{vmatrix} e_1 + e_4 & -e_1 & 0 \\ -e_1 & e_1 + e_2 + e_5 & -e_2 \\ 0 & -e_2 & e_2 + e_3 \end{vmatrix} = e_1 e_2 e_3 + e_1 e_2 e_4 + e_1 e_2 e_5 \\ + e_1 e_3 e_4 + e_1 e_3 e_5 + e_2 e_3 e_4 \\ + e_2 e_4 e_5 + e_3 e_4 e_5. \end{vmatrix}$$

The determinants of other submatrices of M(e) also have combinatorial interpretations; for example, the non-vanishing terms in the expansion of the determinant of the submatrix obtained by deleting the *i*th and *n*th rows and columns of M(e) correspond to spanning forests of two trees in which nodes *i* and *n* belong to different trees (see, for example, Percival (1953)).

Theorem 5.2 is frequently called Maxwell's Rule (see Maxwell (1892) and, in particular, the appendix to Chapter 6 by the editor J. J. Thompson). Borchardt (1860), however, proved an equivalent result in the course of expressing the resultant of two polynomials in terms of their values at certain points. His expression involved a determinant of the same form as $M_n(e)$; he showed that the determinant equalled a sum of the above type and he determined the number of terms in this expression (see also Dixon (1909)). Sylvester (1857) stated without proof a similar rule for expanding certain determinants called unisignants; Cayley referred to Sylvester's Rule in (1856) and to Borchardt's work in (1889). Kirchhoff (1847) gave a result dual to Theorem 5.2 in which a matrix determined by the cycles of G plays the role of A and the sum is over the products of edges forming the complement of a spanning tree of G (for discussions of these papers see, for example, Muir (1911), Ku (1952), Weinberg (1958a), and Chen (1968)). Brooks, Smith, Stone, and Tutte (1940) gave an inductive proof of Theorem 5.2 that was subsequently extended by Tutte (1948) to directed graphs; we shall describe his more general result later.

Let $p(\lambda)$ denote the characteristic polynomial of M. Kelmans (1965, 966) calls $B(\lambda) = p(-\lambda)/\lambda$ the characteristic polynomial of the graph G; t is easy to see that c(G) = B(0)/n. Kelmans investigates properties of the polynomials $B(\lambda)$ in these and other papers and gives an algorithm for determining $B(\lambda)$ that depends on decomposing G into simpler graphs whose polynomials are easier to determine.

Let $R = [r_{ij}]$ denote an *m* by *m* upper triangular matrix. Nakagawa 1958) gives the following recursive definition of the *foldant* ||R|| of such

a matrix: if m = 1, then $||R|| = r_{11}$ and if m > 1, then

$$R = r_{1m} \begin{vmatrix} r_{11} + r_{2m} & r_{12} + r_{3m} & \cdots & r_{1,m-1} + r_{m,m} \\ 0 & r_{22} & \cdots & r_{2,m-1} \\ \vdots & & \ddots & \vdots \\ 0 & & \cdots & 0 & r_{m-1,m-1} \end{vmatrix}$$
$$+ r_{2m} \begin{vmatrix} r_{11} & r_{12} & \cdots & r_{1,m-1} \\ 0 & r_{22} + r_{3m} & \cdots & r_{2,m-1} + r_{m,m} \\ & & r_{33} & & r_{3,m-1} \\ \vdots & & \ddots & \vdots \\ 0 & & \cdots & 0 & r_{m-1,m-1} \end{vmatrix}$$
$$+ \cdots$$
$$+ r_{m,m} \begin{vmatrix} r_{11} & r_{12} & \cdots & r_{1,m-1} \\ 0 & r_{22} & \cdots & r_{2,m-1} \\ \vdots & \ddots & \vdots \\ 0 & & \cdots & 0 & r_{m-1,m-1} \end{vmatrix}$$

Let B denote the matrix obtained from M(e) by (1) changing the entries on and below the main diagonal to zeros, (2) multiplying each of the remaining entries by -1, and (3) deleting the first column and the last row. Nakagawa shows that the foldant of B equals the tree polynomial of the graph G. One advantage of expanding the foldant of B, as opposed to expanding the determinant $M_n(e)$, is that there are no negative products that arise only to cancel out. If G is the graph in Figure 9, then

$$\begin{split} \|B\| &= \left\| \begin{matrix} e_1 & 0 & e_4 \\ 0 & e_2 & e_5 \\ 0 & 0 & e_3 \end{matrix} \right\| = e_4 \left\| \begin{matrix} e_1 + e_5 & e_3 \\ 0 & e_2 \end{matrix} \right\| + e_5 \left\| \begin{matrix} e_1 & 0 \\ 0 & e_2 + e_3 \end{matrix} \right\| + e_3 \left\| \begin{matrix} e_1 & 0 \\ 0 & e_2 \end{matrix} \right\| \\ &= e_4 \{ e_3(e_1 + e_5 + e_2) + e_2(e_1 + e_5) \} + e_5 e_1(e_2 + e_3) + e_3 e_1 e_2 \\ &= e_1 e_2 e_3 + e_1 e_2 e_4 + e_1 e_2 e_5 + e_1 e_3 e_4 + e_1 e_3 e_5 + e_2 e_3 e_4 \\ &+ e_2 e_4 e_5 + e_3 e_4 e_5. \end{split}$$

We now illustrate how Corollary 5.2.1 has been used to obtain formulas for the number of spanning trees in certain graphs G.

5.4. Applications. The number T(n) of trees with *n* labelled nodes is equal to the number of spanning trees of the complete *n*-graph. If we apply

Corollary 5.2.1 to the complete 4-graph, for example, we find that

$$T(4) = \begin{vmatrix} 3 & -1 & -1 \\ -1 & 3 & -1 \\ -1 & -1 & 3 \end{vmatrix} = \begin{vmatrix} 1 & 1 & 1 \\ -1 & 3 & -1 \\ -1 & -1 & 3 \end{vmatrix} = \begin{vmatrix} 1 & 1 & 1 \\ 0 & 4 & 0 \\ 0 & 0 & 4 \end{vmatrix} = 4^2.$$

The general formula $T(n) = n^{n-2}$ can be proved in the same way, as pointed out by Weinberg (1958b). Weinberg also treated the following two generalizations of this problem.

THEOREM 5.3. If W(n, k) denotes the number of spanning trees of a graph obtained from the complete n-graph by removing k edges no two of which have a node in common, then

$$W(n, k) = (n - 2)^k n^{n-2-k}$$

 $if \ 0 \le 2k \le n.$

There is no loss of generality if we assume the missing edges joined nodes 1 and 2, 3 and 4, ..., and 2k - 1 and 2k. If we apply Corollary 5.2.1 when k = 2 and n = 7 we find that

The general formula is proved in the same way (usually the first step in evaluating these determinants is to add to the first row all the other rows).

THEOREM 5.4. If w(n, k) denotes the number of spanning trees of a graph obtained from the complete n-graph by removing k edges all of which are incident with a given node, then

$$w(n, k) = (n - 1 - k)(n - 1)^{k - 1}n^{n - k - 2}$$

if $0 \le k \le n-1$.

Section -

We may assume the missing edges joined node 1 to nodes 2, 3, ..., k + 1. If we apply Corollary 5.2.1 when k = 3 and n = 7 we find that

$$w(7,3) = \begin{vmatrix} \frac{3}{0} & 0 & 0 & 0 \\ 0 & 5 & -1 & -1 \\ 0 & -1 & 5 & -1 \\ 0 & -1 & 5 & -1 \\ \hline 0 & -1 & -1 & 5 \\ \hline -1 & & -1 & 6 \end{vmatrix}$$
$$= \frac{\begin{vmatrix} 1 & 1 & 1 & 1 & 1 \\ 0 & 5 & -1 & -1 \\ 0 & -1 & 5 & -1 \\ \hline 0 & -1 & 5 & -1 \\ \hline -1 & & 6 & -1 \\ \hline -1 & & 6 & -1 \\ \hline -1 & & 6 & -1 \\ \hline 0 & 5 & -1 & -1 \\ \hline 0 & 5 & -1 & -1 \\ \hline 0 & -1 & 5 & -1 \\ \hline -1 & 5 & -1 \\ \hline 0 & 0 & 7 \end{vmatrix}$$
$$= \frac{7^2 \cdot \begin{vmatrix} 3 & 3 & 3 \\ -1 & 5 & -1 \\ -1 & -1 & 5 \end{vmatrix}}{\begin{vmatrix} 3 & 7^2 & 0 \\ 0 & 0 & 6 \end{vmatrix} = 3 \cdot 6^2 \cdot 7^2.$$

The general formula is proved in the same way.

Fiedler and Sedláček (1958) and Simmonard and Hadley (1959) determined the number T(r, s) of r by s bipartite trees by this method. We may assume the r + s nodes are labelled so that the first r nodes are the dark nodes and the last s nodes are the light nodes. If we apply Corollary 5.2.1 when r = 2 and s = 4, we find that

$$T(2,4) = \begin{vmatrix} 4 & 0 & -1 & \\ 0 & 4 & -1 & \\ \hline & 2 & 0 & 0 & \\ -1 & 0 & 2 & 0 & \\ 0 & 0 & 2 & 0 & \\ \hline & -1 & 0 & 2 & 0 & \\ 0 & 0 & 0 & 2 & \\ \end{vmatrix} = \begin{vmatrix} 1 & 1 & 0 & 0 & 0 & \\ 0 & 4 & -1 & -1 & -1 & \\ \hline & 1 & 0 & 0 & 0 & \\ 0 & 0 & 2 & 0 & \\ \hline & 0 & 0 & 2 & 0 & \\ 0 & 0 & 2 & 0 & \\ \hline & 0 & 0 & 2 & \\ \end{vmatrix} = 2^{3} \cdot 4^{1}.$$

The general formula $T(r, s) = r^{s-1}s^{r-1}$ is proved in the same way.

Corollary 5.2.1 has been applied to a number of classes of graphs whose structure is sufficiently simple for the determinant M_n to be evaluated. Most of the formulas that have been derived this way, however, can be derived by other methods also so we will postpone describing more of these results until later.

5.5. The Matrix Tree Theorem for Directed Graphs. Let D denote a directed graph with $n (\geq 2)$ labelled nodes and b arcs; we assume for the present that each arc joins two distinct nodes but there may be several arcs that join the same pair of nodes. If e_1, e_2, \ldots, e_b are variables identified with the arcs of D, let $C = [c_{ij}]$ denote the n by n matrix in which $-c_{ij}$ equals the sum of the arcs directed from node i to node j (or zero, if there are no such arcs) for $i \neq j$, and c_{ii} equals the sum of the arcs directed from the arcs directed from i to other nodes. Let C_i denote the cofactor of c_{ii} in C; since the row sums of C all vanish it follows that the cofactors of the entries in any given row are all equal. If T is a directed spanning subtree of G rooted at node n, say, then the tree product $\Pi(T)$, as before, is the product of the arcs of T.

The following theorem is due to Tutte (1948); the proof we give here involves some modifications due to Knuth (1968a; p. 578) of Tutte's proof (see also van Aardene-Ehrenfest and de Bruijn (1951), Bott and Mayberry (1954), Fiedler and Sedláček (1958), and Chen (1965, 1966a)).

THEOREM 5.5. If $n \ge 2$, then

$$C_n=\sum \Pi(T),$$

where the sum is over all directed spanning subtrees T of D that are rooted at the nth node.

If some node $i (\langle n \rangle)$ of D has out-degree zero, then every entry in the *i*th row of C is zero and there are no directed spanning subtrees T of D that are rooted at node n. Hence $C_n = 0 = \sum \Pi(T)$ in this case.

We next consider the case in which each of the first n - 1 nodes has out-degree one and the *n*th node has out-degree zero. If *D* is not a directed tree, then some subset of the first n - 1 nodes determines a connected component; the sum of the columns of *C* corresponding to these nodes vanishes, so $C_n = 0 = \sum \prod(T)$ again. Suppose *D* is a directed tree (rooted at node *n*); if the nodes of *D* are relabelled (this amounts to simultaneously permuting rows and columns of *C*) according to the order in which they would be removed in determining the Prüfer sequence associated with the tree, then *C* becomes an upper triangular matrix and C_n equals the tree product of *D*.

It remains to consider the case in which the first n - 1 nodes all have positive out-degree and there is some node, say the 1st, whose out-degree exceeds one. If e denotes some arc directed from node 1 to some other node, say node 2, let E and F denote the matrices obtained by suppressing the e's, and all variables except the e's, in the first row of C. The matrices E and F correspond to the graphs obtained from D by deleting arc e and by deleting all arcs except e that lead away from the 1st node. These graphs both have fewer edges than D so we may assume E_n and F_n enumerate their spanning subtrees that are rooted at node n. It is not difficult to see that E_n enumerates those spanning subtrees of D rooted at node nthat do not contain arc e while F_n enumerates those that do. Since $C_n =$ $E_n + F_n$, the required result now follows by induction on the number of arcs of D.

The spanning subtrees of D that are rooted at node i are enumerated by the cofactor C_i ; it is not difficult to reformulate the statement of Theorem 5.5 so as to enumerate the rooted spanning subtrees of D whose arcs are all directed away from the root. A directed graph D is balanced if for each node i there are an equal number of arcs directed away from and towards i. If D is balanced then the column sums of the matrix obtained from C by replacing the e's by 1's all vanish; hence all the cofactors are equal and the number of spanning subtrees of D is independent of the root node. If Dis symmetric, that is, if the arc ij is in D if and only if the arc ji is in D, then

Theorem 5.5 reduces, in effect, to Theorem 5.2. Knuth (1968b) shows that Theorem 5.5 can also be used to derive Theorem 2.2.

5.6. Trees in the Arc-Graph of a Directed Graph. The arc-graph A = A(D) of a directed graph D is the directed graph whose nodes N(i, j) correspond to the arcs ij of D and in which an arc is directed from N(i, j) to N(k, h) if and only if j = k (see Figure 10). If there are w_i arcs of the type ij in D and l_i of the type ki, then A has $w_1 + \cdots + w_n = l_1 + \cdots + l_n$ nodes and $w_1l_1 + \cdots + w_nl_n$ arcs. If $l_i = 0$ there are no





nodes of the type N(k, i) in A. Let D' denote the graph obtained from D by removing all nodes i such that $l_i = 0$ (and all arcs of the type ij). We may suppose D' is the subgraph determined by the first m nodes of D (in the example, m = 3). Knuth (1967) used Theorem 5.5 to express the number of spanning subtrees of A(D) rooted at a given node N(u, v) in terms of the numbers t_y of spanning subtrees of D' rooted at various nodes y.

THEOREM 5.6. There are

$$w_1^{l_1-1}\cdots w_m^{l_m-1}(t_v - w_v^{-1}\sum t_v)$$

spanning subtrees of A(D) rooted at node N(u, v), where the sum is over all nodes y of D' such that $y \neq u$ and the arc yv is in D'.

Let the matrices C(A) and C = C(D') be defined as before for the graphs A and D' except that all the variables are replaced by 1's (we ignore any loops the graphs may have in defining these matrices). We may assume the nodes of A are grouped together so that C(A) can be expressed as an m by m array of submatrices B_{jk} , where if $j \neq k$ the entries of B_{jk} indicate the arcs directed from nodes N(i, j) to nodes N(k, h); we may also assume v = 1 and that the first row and column of C(A) correspond to the root

N(u, v). If A is the arc-graph in Figure 10 rooted at node N(2, 1), then

	2	0	0	-1	0	-1	0
	0	2	0	-1	0	-1	0
	0	0	2	-1	0	-1	0
C(A) =	-1	0	0	1	0	0	0
	-1	0	0	0	1	0	0
	0	-1	0	0	-1	3	-1
	0	-1	0	0	-1	0	2

Notice that when $j \neq k$ each column of B_{jk} consists entirely of 0's or -1's and that there are $-c_{jk}$ columns of the latter type where $-c_{jk}$ denotes the number of arcs directed from j to k in D'.

Let C^* denote the matrix obtained from C(A) by adding the column $(\lambda, 0, ..., 0)$ to the first column of C for some indeterminate λ . Since det C(A) = 0, it follows that det $C^* = \lambda C_1(A)$, where the cofactor $C_1(A)$ of the first entry in C(A) is the required number of spanning trees of A. It remains, therefore, to evaluate the determinant of C^* .

Add to the first column of each submatrix B_{jk} of C^* all the remaining columns of B_{jk} and then subtract the first row of each submatrix B_{jk} from the remaining rows of B_{jk} . It is not difficult to see that these transformed submatrices B_{jk} now have the form

					$c_{kk} + \lambda \delta_{k1}$	-		• • •		-	
	c_{jk} –	•••	-		$-\lambda\delta_{k1}$	w_k	0	• • •		0	
$B_{jk} =$	0	•••	0	or $B_{kk} =$		0				:	
			:		•	÷		۰.		0	
	10	• • •	0		$-\lambda \delta_{k1}$	0		• • •	0	w_k	

according as $j \neq k$ or j = k; the dashes indicate entries left unspecified for the present. (To establish the second expression recall that the original submatrix B_{kk} has a -1 in an off-diagonal position only if the column corresponds to a loop in D'; the number c_{kk} equals w_k minus the number of loops at the kth node of D'.)

If we apply these steps to the example considered earlier we find that



	2 +	λ	0	0	-1	i — 1	L
	-λ		2	0	() ()
= 1.3	-λ		0	2	() ()
	-1		0	0	1	L ()
	-1		1	0	-1	1 2	2
	λ	0		0	-1	-1	1
	$-\lambda$	2		0	0	0	
$= 1 \cdot 3$	$-\lambda$	0		2	0	0	,
	0	0		0	1	0	
	0	-1		0	-1	2	

where we have factored out diagonal entries that are the only non-zero entry in their rows, removed the corresponding rows and columns, and then added the last m - 1 = 2 columns to the first column. In the general case we find that

	λ	-		•••		-	c_{12}	•••	c_{1m}	
	$-\lambda$	w_1	0	• • •		0	0	• • •	0	
		0				÷	:		:	
$\det C^* = w_2^{l_2-1} \cdots w_m^{m-1}$	÷	÷		••.		0				
	$-\lambda$	0		•••	0	w_1	0	•••	0	
	0	-		• • •		-	c_{22}	• • •	<i>C</i> _{2m}	
	÷	÷				÷	:		:	
	0	-		•••		-	c_{m2}	•••	c_{mm}	

The unspecified entries in the column corresponding to a node of the type N(y, 1), where $y \neq u$, are all zero except when y is a node of D' in which case there is a -1 in the row in which c_{y2}, \ldots, c_{ym} appear. Hence, if we expand the last determinant along the first column we find that

$$\lambda C_1(A) = \det C^* = w_1^{l_1-1} \cdots w_m^{l_m-1} \Big\{ \lambda w_1^{l_1-1} C_{11} - \lambda w_1^{l_1-2} \sum C_{y1} \Big\},$$

where C_{y1} denotes the cofactor of c_{y1} in the matrix C of D' and the sum is over all nodes y in D' such that $y \neq u$ and the arc y1 is in D'. This suffices to complete the proof of the theorem, since it follows from Theorem 5.5 that $C_{11} = t_v$ and $C_{y1} = C_{yy} = t_y$.

If the digraph D is balanced then the formula in Theorem 5.6 simplifies to $w_1^{w_1-1} \cdots w_m^{w_m-1} t/w_v$, where t is the number of spanning subtrees of D'with a given root; if D is *regular* of degree d, that is, if $w_i = d = l_i$ for all i, the formula simplifies further to $td^{n(d-1)-1}$. An Eulerian circuit of a directed graph D is a directed cycle that contains every arc of D just once. It is not difficult to show that a connected balanced directed graph D has $t \cdot \prod_{i=1}^{n} (w_i - 1)!$ Eulerian circuits, where tdenotes the number of spanning trees of D rooted at any given node (see van Aardene-Ehrenfest and de Bruijn (1951), Smith and Tutte (1941), and Baum and Eagon (1966)). Knuth (1967) used this result and Theorem 5.6 to give another derivation of the result due to van Aardene-Ehrenfest and de Bruijn that if the directed graph D is regular of degree d, then A(D) has $d^{-1}(d!)^{n(d-1)}$ times as many Eulerian circuits as D.

5.7. Listing the Trees in a Graph. Feussner (1902, 1904) gave a method for listing the spanning trees of a graph G that is based upon the fact that any spanning tree either does or does not contain a given edge e. Let G' denote the graph obtained from G by removing edge e and let G" denote the graph obtained from G by removing all edges that join the endnodes of e and then identifying the endnodes of e. The graphs G' and G" are simpler than G and the tree polynomial of G equals the tree polynomial of G' plus e times the tree polynomial of G". This process can be repeated until the trees can be determined by inspection (notice that the tree polynomial of a graph equals the product of the tree polynomials of its blocks). If we use this method to determine the number $c(\langle 4 \rangle)$ of trees spanning the complete 4-graph, we find that

$c\left(\bigtriangleup\right) = c\left(\swarrow\right) + c\left(\Box\right)$	
$= c \left($)
$= 4 + 2 \cdot 2^2 + 4 = 16.$	

The idea upon which Feussner's method is based can also be exploited to prove various results, such as Theorems 5.2 and 5.5 and Nakagawa's foldant algorithm, by induction on the size of the graph. Many papers have been written giving algorithms, of varying degrees of usefulness, for listing the spanning trees of a graph; a small fraction of them, for example, are those by Wang (1934), Duffin (1959), Hakimi (1961), Mayeda and Seshu (1965), Mukherjee and Sarker (1966), Chen (1966b), Berger (1967), and Char (1968).

THE METHOD OF INCLUSION

AND EXCLUSION

6

6.1. Introduction. The method of inclusion and exclusion can be used to express the number of spanning trees of a given graph G in terms of the number of trees that contain different subsets of edges that do not belong to G. In this section we illustrate this approach on various problems where the expressions obtained are reasonably manageable. Some of the material in the first part of this chapter was presented at a course on "Graph Theory and its Uses" at the London School of Economics in July, 1964 and appeared in Moon (1967b).

6.2. The Number of Trees Spanned by a Given Forest. Any spanning subgraph of a tree T_n is a forest F_n of one or more disjoint trees. Let $l = l(F_n)$ denote the number of components of F_n (some of which may be isolated nodes) and let $p = p(F_n)$ denote the product of the number of nodes in the *l* components of F_n . The following useful result shows that the number $T(F_n)$ of trees T_n that contain a given forest F_n depends only on the size of the components of F_n and not on their individual structure.

THEOREM 6.1. $T(F_n) = p(F_n)n^{l(F_n)-2}$.

Suppose the components of F_n are labelled from 1 to l (in the order, say, of the size of the smallest label associated with the nodes of each component) and suppose the *i*th component has j_i nodes where $j_1 + j_2 + \cdots + j_i = n$. Pretend, for a moment, that each component is a node by itself and construct a tree T_l with degree-sequence (d_1, d_2, \ldots, d_l) on these l nodes. To transform T_l into a tree T_n containing F_n , we replace each of the d_i edges incident with the *i*th node of T_l by an edge incident with one of the j_i nodes of the *i*th component of F_n , for each *i*. If we carry out these operations in all possible ways, then it follows from Theorem 3.1 and the **52**

multinomial theorem that

$$T(F_n) = \sum {\binom{l-2}{d_1-1,\ldots,d_l-1}} j_1^{d_1} \cdots j_l^{d_l}$$

= $j_1 \cdots j_l (j_1 + \cdots + j_l)^{l-2} = pn^{l-2}.$

Notice that the formula reduces to n^{n-2} when F_n consists of n isolated nodes. Glicksman (1963) and Knuth (1968b) have proved an equivalent result involving mapping functions. Glicksman's proof is by induction and uses ideas similar to those used by Göbel in the proof of Theorem 3.3; Knuth's proof is by an extension of Prüfer's method. Sedláček (1966) used matrix methods to prove the special case when only one component of F_n has more than one node (in (1967) he used this case to give a combinatorial proof of an identity involving binomial coefficients; in this paper he also showed that if node x has degree β in the connected graph G and belongs to α blocks, then G has a spanning tree in which x has degree k for any integer k such that $\alpha \leq k \leq \beta$).

Theorem 6.1 can be used, for example, to give alternate derivations of Weinberg's formulas in Theorems 5.3 and 5.4. To prove Theorem 5.3 notice that if the forest F_n consists of t edges no two of which have a node in common and n - 2t isolated nodes, then $T(F_n) = 2^t n^{n-t-2}$. Hence, if W(n, k) denotes the number of spanning trees of a graph obtained from the complete *n*-graph by removing k edges no two of which have a node in common, it follows from the method of inclusion and exclusion that

$$W(n,k) = n^{n-2} - k2n^{n-3} + {\binom{k}{2}}2^2n^{n-4} - \cdots$$
$$= n^{n-2}\sum_{t=0}^{k} {\binom{k}{t}} {\binom{-2}{n}^t} = n^{n-2} {\binom{1-\frac{2}{n}^k}{n}^t}$$

if $0 \leq 2k \leq n$.

To prove Theorem 5.4 notice that if the forest F_n consists of t edges incident with the same node and n - (t + 1) isolated nodes, then $T(F_n) = (t + 1)n^{n-t-2}$. Hence, if w(n, k) denotes the number of spanning trees of a graph obtained from the complete *n*-graph by removing k edges incident with a given node, then

$$w(n, k) = n^{n-2} - k2n^{n-3} + \binom{k}{2} 3n^{n-4} - \cdots$$

= $n^{n-2} \sum_{t=0}^{k} (t+1)\binom{k}{t} \left(\frac{-1}{n}\right)^{t}$
= $n^{n-2} \left\{ -\frac{t}{n} \left(1 - \frac{1}{n}\right)^{k-1} + \left(1 - \frac{1}{n}\right)^{k} \right\}$
= $n^{n-2} \left(1 - \frac{k+1}{n}\right) \left(1 - \frac{1}{n}\right)^{k-1}$

 $\text{if } 0 \leq k \leq n-1.$

54 The Method of Inclusion and Exclusion

6.3. The Number of Spanning Trees of a Graph. This approach can be used, in principle, to determine the number c(G) of spanning trees of any (connected) graph G. If H_m is any graph with m labelled nodes and n is any positive integer, let

(6.1)
$$f(H_m, n) = \sum p(F_m)(-n)^{l(F_m)-m}$$

where the sum is over all spanning forests F_m of H_m (notice that $m - l(F_m)$ is the number of edges in F_m); it follows from this definition that if the connected components of the graph H are A, B, \ldots , then

$$f(H, n) = f(A, n)f(B, n) \dots$$

The complement of a graph G_n is the graph \overline{G}_n obtained from the complete *n*-graph by removing all edges that appear in G_n . The following general formula follows readily from Theorem 6.1 and the method of inclusion and exclusion.

THEOREM 6.2. $c(G_n) = n^{n-2} f(\overline{G}_n, n).$

Temperley (1964) obtained this result by applying a transformation to the matrix in Theorem 5.2. Bedrosian (1964b) stated that $c(G_n)$ equals n^{n-2} times a product of factors associated with the components of \overline{G}_n and he gave formulas for the factors associated with certain graphs.

6.4. Examples. One nice feature of Theorem 6.2 is that once the polynomials f have been evaluated for a collection X of graphs (this is the hard part), then one can immediately give formulas for the number of trees spanning any graph G the components of whose complement belong to X. We now determine the polynomials $f(H_m, n)$ for a few classes of graphs H_m ; it is usually convenient to express $f(H_m, n)$ as a double sum, where the outer sum is over the exponent of n and the inner sum is over all spanning forests with the appropriate number of components (or edges).

THEOREM 6.3. If $\langle m \rangle$ denotes the complete m-graph, then

$$f(\langle m \rangle, n) = \left(1 - \frac{m}{n}\right)^{m-1}.$$

If we apply the definition of $f(\langle m \rangle, n)$ and use identity (3.4) we find that

$$f(\langle m \rangle, n) = \sum_{l=1}^{m} (-n)^{l-m} \frac{1}{l!} \sum {\binom{m}{j_1, \dots, j_l}} j_1^{j_1-1} \cdots j_l^{j_l-1}$$
$$= \sum_{l=1}^{m} {\binom{m-1}{l-1}} \left(-\frac{m}{n}\right)^{m-l} = \left(1-\frac{m}{n}\right)^{m-1}.$$

The complete k-partite graph $\langle c_1, \ldots, c_k \rangle$ consists of c_i nodes of colour

i, for i = 1, 2, ..., k, and all edges of the type xy where nodes x and y have different colours. The following result follows from Theorems 6.2 and 6.3.

COROLLARY 6.3.1. If
$$c_1 + c_2 + \cdots + c_k = n$$
, then

$$c(\langle c_1,\ldots,c_k\rangle)=n^{k-2}\prod_{i=1}^k(n-c_i)^{c_i-1}.$$

This formula was apparently derived first by Austin (1960) who used the result in Corollary 5.2.1; Good (1965) used a multivariate generating function to give another derivation and Oláh (1968) gave a proof based on Prüfer's method. Notice that when k = 2 this reduces to the formula derived earlier for the number of bipartite trees.

THEOREM 6.4. If $\langle r, s \rangle$ denotes the complete r by s bipartite graph, then

$$f(\langle r,s\rangle,n)=\left(1-\frac{r}{n}\right)^{s-1}\left(1-\frac{s}{n}\right)^{r-1}\left(1-\frac{r+s}{n}\right)^{r-1}$$

If F(r, s; k, l) denotes the number of r by s bipartite forests of k + l trees k of which are rooted at a dark node and l at a light node, then it follows from the definition of $f(\langle r, s \rangle, n)$ and equation (4.7) that

$$f(\langle r, s \rangle, n) = \sum_{t=1}^{r+s} (-n)^{t-r-s} \sum_{k+l=t} F(r, s; k, l)$$

= $\sum_{t=1}^{r+s} (-n)^{t-r-s} \sum_{k+l=t} {r \choose k} {s \choose l} (rl + sk - kl) r^{s-l-1} s^{r-k-1}$
= $\sum_{n=0}^{r+s-1} \sum_{i+j=n} {r \choose i} {s \choose j} \left(-\frac{r}{n}\right)^{j-1} \left(-\frac{s}{n}\right)^{i-1} \left(\frac{rs}{n^2} - \frac{ij}{n^2}\right)$
= $\left(1 - \frac{r}{n}\right)^s \left(1 - \frac{s}{n}\right)^r - \frac{rs}{n^2} \left(1 - \frac{r}{n}\right)^{s-1} \left(1 - \frac{s}{n}\right)^{r-1}$
= $\left(1 - \frac{r}{n}\right)^{s-1} \left(1 - \frac{s}{n}\right)^{r-1} \left(1 - \frac{r+s}{n}\right)$.

If we apply Theorems 6.2 and 6.4 to determine $c(G_n)$ when the components of \overline{G}_n are either complete bipartite graphs or isolated nodes, we obtain a formula O'Neil and Slepian (1966) established by evaluating the appropriate determinant. Notice that Weinberg's formulas for W(n, k) and w(n, k) also follow from Theorems 6.2 and 6.4. O'Neil, in a letter dated March, 1969, states that he has generalized Theorems 6.3 and 6.4 by 3+c.t.T.

showing, in effect, that if $c_1 + c_2 + \cdots + c_k = m$, then

$$f(\langle c_1,\ldots,c_k\rangle,n)=\left(1-\frac{m}{n}\right)^{k-1}\prod_{i=1}^{k}\left(1-\frac{m-c_i}{n}\right)^{c_i-1};$$

this formula can be derived using Corollary 2.3.3.

THEOREM 6.5. If P_m denotes a path of length m - 1, then

$$f(P_m, n) = \sum_{e=0}^{m-1} {\binom{2m-1-e}{e}} {\left(-\frac{1}{n}\right)^e}$$

Every component of a forest F_m spanning P_m is itself a path. It is not difficult to see that the sum $\sum p(F_m)$, taken over all spanning forests F_m of P_m such that $l(F_m) = l$, equals the coefficient of x^m in

$$(x + 2x^{2} + 3x^{3} + \cdots)^{l} = [x(1 - x)^{-2}]^{l}.$$

Therefore

$$f(P_m, n) = \sum_{l=1}^{m} {\binom{m+l-1}{m-l}} \left(-\frac{1}{n}\right)^{m-l} = \sum_{e=0}^{m-1} {\binom{2m-1-e}{e}} \left(-\frac{1}{n}\right)^{e}$$

THEOREM 6.6. If C_m denotes a cycle of length m, then

$$f(C_m, n) = \sum_{e=0}^{m-2} \sum_{j=1}^{e+1} j^2 \binom{2m-2-e-j}{e+1-j} (-n)^{-e} + m^2 (-n)^{1-m}.$$

Every component of a forest F_n spanning C_m is a path. Suppose we label the components of F_n beginning with the component containing an arbitrary node u and proceeding along the cycle in the clockwise sense. The sum $\sum p(F_m)$, taken over all spanning forests F_m of C_m such that $l(F_m) = l$, is equal to

$$\sum j_1(j_1j_2\cdots j_l)$$

summed over all compositions of m into l positive integers (the extra factor j_1 arises from the fact that the node u could be any of the j_1 nodes in the first component of F_m). When l = 1, the expression equals m^2 ; when l > 1 we can set $j_1 = j$ and sum over the remaining factors. This latter sum is the same as the sum we considered in the proof of Theorem 6.5 except that m and l are replaced by m - j and l - 1. Therefore,

$$f(C_m, n) = m^2(-n)^{1-m} + \sum_{l=2}^m \sum_{j=1}^{m-l+1} \binom{m-j+l-2}{m-j-l+1} (-n)^{l-m}.$$

If we let e = m - l this becomes the formula given above.

Bercovici (1969) has shown that

$$f(C_m, n) = \frac{1}{n^m} \begin{vmatrix} n-2 & 1 & 0 & \cdots & 0 & 1 \\ 1 & n-2 & 0 & & 0 \\ 0 & 1 & n-2 & 1 & & \vdots \\ \vdots & & & \ddots & & \\ \vdots & & & & 0 \\ 0 & & & & 1 \\ 1 & 0 & & \cdots & 0 & 1 & n-2 \end{vmatrix}$$
$$= \prod_{k=1}^{m-1} \left\{ 1 - \frac{4}{n} \sin^2\left(\frac{k\pi}{m}\right) \right\},$$

where the matrix has m rows and columns. If $\rho(m) = f(P_{m+1}, n)$, then he has also shown that

$$\rho(a + b) = \rho(a)\rho(b) - \frac{1}{n^2}\rho(a - 1)\rho(b - 1);$$

this implies that

$$\rho(a+1) = \left(1 - \frac{2}{n}\right)\rho(a) - \frac{1}{n^2}\rho(a-1),$$

$$\rho(2a) = \rho^2(a) - \frac{1}{n^2}\rho(a-1),$$

and

$$\rho(2a + 1) = \rho(a) \Big\{ 2\rho(a + 1) - \Big(1 - \frac{2}{n}\Big)\rho(a) \Big\}$$

(He has also given analogous recurrence relations for the polynomials of graphs obtained from the graphs $\langle 1, 3 \rangle$ or $\langle 1, 4 \rangle$ by inserting additional nodes in the edges so as to form more edges.) The first few polynomials for paths and cycles are given in Table 2. Bedrosian (1970) pointed out that $(n - 4) f^2 (P_{m,n}) = f (C_{2m,n})$.

TABLE 2							
m	$n^{m-1}f(P_m,n)$	$n^{m-1}f(C_m, n)$					
2	n-2						
3	(n-1)(n-3)	$(n-3)^2$					
4	$(n-2)(n^2-4n+2)$	$(n-2)^2(n-4)$					
5	$(n^2 - 3n + 1)(n^2 - 5n + 5)$	$(n^2 - 5n + 5)^2$					
6	$(n-1)(n-2)(n-3)(n^2-4n+1)$	$(n-1)^2(n-3)^2(n-4)$					

Bedrosian (1961, 1964b) derived formulas for $f(P_m, n)$ and $f(C_m, n)$ using the foldant algorithm of Nakagawa (1958) and he has expressed these polynomials in terms of a third family of polynomials the absolute values of whose coefficients add up to a Fibonacci number. Bedrosian (1964b) and Ku and Bedrosian (1965) consider the problem of determining the polynomial of a subgraph I of a graph H when the polynomials of H and the complement of I in H are known; they state, for example, that if $\{m, h\}$ denotes the graph obtained from a complete m-graph by removing edges that form a complete h-graph, then

$$f(\{m, h\}, n) = \left(1 - \frac{m-h}{n}\right)^{h-1} \left(1 - \frac{m}{n}\right)^{m-h}$$

if $h \le m$. They also consider analogous enumeration problems for graphs in which several edges may join the same pair of nodes.

If A and B are two disjoint graphs with a + 1 and b + 1 nodes, respectively, let $A \circ B$ denote a graph obtained by identifying some node of A with some node of B; we shall let x denote the node common to A and B in $A \circ B$. Kasai *et al.* (1966a) used matrix methods to determine c(G) when \overline{G} consists of isolated nodes and one of ten types of graphs $A \circ B$ where A and B are complete graphs, cycles, paths or complete 1 by s bipartite graphs (in a subsequent paper (1966b) they discussed the use of continuants in evaluating determinants that arise in these problems). The formulas that arise when A or B are paths or cycles are rather complicated so we shall derive polynomials of $A \circ B$ only when A and B are complete graphs $\langle m \rangle$ or complete bipartite graphs $\langle 1, s \rangle$.

For some of these problems it is slightly more convenient to consider a graph $A \oplus B$ obtained by joining a node x in A to a node y in B. Some examples of graphs $A \circ B$ and $A \oplus B$ are given in Figure 11.



FIGURE 11

If T and A are two graphs, let A - T denote the subgraph determined by the nodes of A that do not belong to T and let $\gamma(T)$ denote the number of nodes in the graph T. To determine $f(A \oplus B, n)$ we shall use the fact that

(6.2)
$$f(A \oplus B, n) = f(A, n)f(B, n)$$

+ $\sum \gamma(T)(-n)^{1-\gamma(T)}f(A - T, n)f(B - T, n),$

where the sum is over all subtrees T of $A \oplus B$ that contain the edge xy; this follows immediately from the definition of $A \oplus B$ and the polynomials f.

THEOREM 6.7. If $A = \langle 1, a \rangle$, $B = \langle 1, b \rangle$, and $A \oplus B$ is the graph obtained by joining the dark node x of A to the dark node y of B, then

$$f(A \oplus B, n) = \left(1 - \frac{1}{n}\right)^{a+b-2} \left\{ \left(1 - \frac{1}{n}\right)^2 \left(1 - \frac{a+b+2}{n}\right) + \frac{ab}{n^2} \right\}$$

There are $\binom{a}{i}\binom{b}{j}$ subtrees T of $A \oplus B$ that contain the edge xy and i additional nodes of A and j additional nodes of B (see Figure 11). It follows, therefore, from (6.2) and Theorem 6.4 that

$$f(A \oplus B, n) = f(A, n)f(B, n) + \sum_{i,j} {a \choose j} {b \choose j} (i + j + 2)(-n)^{-1 - i - j}$$

= $f(A, n)f(B, n)$
+ $\sum_{i} {a \choose i} (-n)^{-1 - i} \left\{ (i + 2) \left(1 - \frac{1}{n}\right)^{b} - \frac{b}{n} \left(1 - \frac{1}{n}\right)^{b - 1} \right\}$
= $\left(1 - \frac{1}{n}\right)^{a - 1} \left(1 - \frac{a + 1}{n}\right) \left(1 - \frac{1}{n}\right)^{b - 1} \left(1 - \frac{b + 1}{n}\right)$
 $- n^{-1} \left(1 - \frac{1}{n}\right)^{b - 1} \left\{ \left(2 - \frac{b + 2}{n}\right) \left(1 - \frac{1}{n}\right)^{a} - \frac{a}{n} \left(1 - \frac{1}{n}\right)^{a} \right\}$

This last expression equals the right hand side of the required formula. We shall need the identities

(6.3)
$$\sum_{l=0}^{m} {m \choose l} (l+1)^{l-1} (-n)^{-l} \left(1 - \frac{m-l}{n}\right)^{m-l-1} = \left(1 - \frac{1}{n}\right) \left(1 - \frac{m+1}{n}\right)^{m-1}$$

(6.4)
$$\sum_{l=0}^{m} {m \choose l} (l+1)^{l} (-n)^{-l} \left(1 - \frac{m-l}{n}\right)^{m-l-1} = \left(1 - \frac{m+1}{n}\right)^{m}$$

in proving the next three theorems; they follow from the first two identities in Table 1.

THEOREM 6.8. If $A = \langle 1, a \rangle$, $B = \langle b + 1 \rangle$, and $A \oplus B$ denotes the graph obtained by joining the dark node x of A to any node y of B, then

$$f(A \oplus B, n) = \left(1 - \frac{1}{n}\right)^{a-1} \left(1 - \frac{b+1}{n}\right)^{b-1} \\ \times \left\{ \left(1 - \frac{a+1}{n}\right) \left(1 - \frac{b+1}{n}\right) - \frac{1}{n} \left(1 - \frac{1}{n}\right) \left(2 - \frac{a+b+2}{n}\right) \right\}.$$

There are $\binom{a}{i}\binom{b}{j}(j+1)^{j-1}$ subtrees T of $A \oplus B$ that contain the edge xy and i additional nodes of A and j additional nodes of B (see Figure 11). It follows, therefore, from Theorems 6.3 and 6.4 and equations (6.2)–(6.4) that

$$f(A \oplus B, n) = f(A, n)f(B, n) + \sum_{i,j} {a \choose i} {b \choose j}$$

$$\times (j+1)^{j-1}(i+j+2)(-n)^{-1-i-j} \left(1 - \frac{b-j}{n}\right)^{b-j-1}$$

$$= f(A, n)f(B, n) + \sum_{i} {a \choose i}(-n)^{-1-i}$$

$$\times \left\{ (i+1) \left(1 - \frac{1}{n}\right) \left(1 - \frac{b+1}{n}\right)^{b-1} + \left(1 - \frac{b+1}{n}\right)^{b} \right\}$$

$$= \left(1 - \frac{1}{n}\right)^{a-1} \left(1 - \frac{a+1}{n}\right) \left(1 - \frac{b+1}{n}\right)^{b}$$

$$- \frac{1}{n} \left(1 - \frac{1}{n}\right)^{a} \left(1 - \frac{b+1}{n}\right)^{b-1} \left(2 - \frac{b+2}{n}\right)$$

$$+ \frac{a}{n^{2}} \left(1 - \frac{1}{n}\right)^{a} \left(1 - \frac{b+1}{n}\right)^{b-1}.$$

This last expression equals the right hand side of the required formula. The next two cases were not among the ten considered by Kasai *et al.* (1966a), but they can be treated in much the same way as were the last two.

THEOREM 6.9. If
$$A = \langle a + 1 \rangle$$
 and $B = \langle b + 1 \rangle$, then
 $f(A \oplus B, n) = \left(1 - \frac{a+1}{n}\right)^{a-1} \left(1 - \frac{b+1}{n}\right)^{b-1}$
 $\times \left\{ \left(1 - \frac{a+1}{n}\right) \left(1 - \frac{b+1}{n}\right) - \frac{1}{n} \left(1 - \frac{1}{n}\right) \left(2 - \frac{a+b+2}{n}\right) \right\}.$

There are $\binom{a}{i}\binom{b}{j}(i+1)^{i-1}(j+1)^{j-1}$ subtrees of $A \oplus B$ that contain the edge joining A and B and i additional nodes of A and j additional nodes of B. Hence,

$$f(A \oplus B, n) = \left(1 - \frac{a+1}{n}\right)^{a} \left(1 - \frac{b+1}{n}\right)^{b}$$
$$+ \sum_{i,j} {a \choose i} {b \choose j} (i+1)^{i-1} (j+1)^{j-1} (i+j+2) (-n)^{-1-i-j}$$
$$\times \left(1 - \frac{a-i}{n}\right)^{a-i-1} \left(1 - \frac{b-j}{n}\right)^{b-j-1}$$

by (6.2) and Theorem 6.8. This expression can be reduced to the stated formula by much the same procedure as was used in proving Theorem 6.8 except that now identities (6.3) and (6.4) must be used twice each.

To determine $f(A \circ B, n)$ we shall use the fact that

(6.5)
$$f(A \circ B, n) = \sum \gamma(T)(-n)^{1-\gamma(T)}f(A - T, n)f(B - T, n),$$

where the sum is over all subtrees T of $A \circ B$ that contain the node x; this follows immediately from the definition of $f(A \circ B, n)$. Notice that this implies relation (6.1) when node x is joined only to one other node of A or of B. The next result was stated by Bedrosian (1964b).

THEOREM 6.10. If $A = \langle 1, a \rangle$, $B = \langle b + 1 \rangle$, and $A \circ B$ is the graph obtained by identifying the dark node x of A with any node of B, then

$$f(A \circ B, n) = \left(1 - \frac{1}{n}\right)^{a} \left(1 - \frac{b+1}{n}\right)^{b-1} \left(1 - \frac{a+b+1}{n}\right)^{b-1}$$

There are $\binom{a}{i}\binom{b}{j}(j+1)^{j-1}$ subtrees of $A \circ B$ that contain the node x and *i* additional nodes of A and *j* additional nodes of B. It follows, therefore, from (6.5) and Theorem 6.3 that

$$f(A \circ B, n) = \sum_{i,j} {\binom{a}{i}} {\binom{b}{j}} (j+1)^{j-1} (i+j+1) (-n)^{-i-j} \left(1 - \frac{b-j}{n}\right)^{b-j-1}.$$

This expression is similar to an expression occurring in the proof of Theorem 6.8 and it can be simplified in the same way.

THEOREM 6.11. If $A = \langle a+1 \rangle$ and $B = \langle b+1 \rangle$, then $f(A \circ B, n) = \left(1 - \frac{1}{n}\right) \left(1 - \frac{a+1}{n}\right)^{a-1} \left(1 - \frac{b+1}{n}\right)^{b-1} \left(1 - \frac{a+b+1}{n}\right).$ There are $\binom{a}{i} \binom{b}{j} (i+1)^{i-1} (j+1)^{j-1}$ subtrees of $A \circ B$ that contain the 3^*

node x and i additional nodes of A and j additional nodes of B. Hence,

$$f(A \circ B, n) = \sum_{i,j} {a \choose i} {b \choose j} (i+1)^{i-1} (j+1)^{j-1} (i+j+1) (-n)^{-i-j} \times \left(1 - \frac{a-i}{n}\right)^{a-i-1} \left(1 - \frac{b-j}{n}\right)^{b-j-1}$$

This expression is similar to an expression occurring in the proof of Theorem 6.9 and it can be simplified in the same way.

Kasai *et al.* (1966a) refer to some earlier papers in which some of their formulas appear and they say they have considered the corresponding problem for graphs formed from two complete graphs or two cycles that have more than one node in common.

6.5. Trees Containing a Given Number of Specified Edges. In the last few results we have been counting trees that do not contain any edges from certain sets of edges; the same kind of argument can be applied, in principle, to count trees that contain a given number of edges from certain sets of edges.

Let *H* denote a graph with *n* labelled nodes and *c* connected components whose *i*th component has m_i nodes. If $E = (e_1, \ldots, e_c)$ denotes a sequence of *c* integers such that $0 \le e_i \le m_i - 1$ for each *i*, let T(H, E) denote the number of trees T_n that contain e_i edges that belong to the *i*th component of *H*, and $n - 1 - \sum e_i$ edges that join nodes that belong to different components of *H*, for $i = 1, 2, \ldots, c$. If $0 \le e \le m - 1$ and H_m is a connected graph with *m* nodes, let

(6.6)
$$f(H_m, e, n) = \sum (-1)^e \binom{m - l(F_m)}{e} p(F_m) (-n)^{l(F_m) - m}$$

where the sum is over all spanning forests F_m of H_m . It follows from the method of inclusion and exclusion that

(6.7)
$$T(H, E) = n^{n-2} f(A, e_1, n) f(B, e_2, n) \dots,$$

where the product is over the c components of H; notice that this reduces to Theorem 6.2 when E = (0, 0, ..., 0) and H is the complement of the graph G whose spanning trees are to be counted.

We now give a closed expression for f(H, e, n) for three classes of connected graphs; in most cases these polynomials are too complicated to be determined explicitly.

THEOREM 6.12. If $0 \le e \le m - 1$ and $H = \langle 1, m \rangle$, then

$$f(H, e, n) = n^{e} {\binom{m}{e}} \left(1 - \frac{1}{n}\right)^{m-e-1} \left(e + 1 - \frac{m+1}{n}\right).$$

There are $\binom{m}{h}$ spanning forests F of $\langle 1, m \rangle$ that have m - h + 1 components and h edges, and p(F) = h + 1 for each such forest. Hence,

$$f(H, e, n) = \sum_{h=e}^{m} (-1)^{e} {\binom{h}{e}} {\binom{m}{h}} (h+1)(-n)^{h}$$
$$= n^{e} {\binom{m}{e}} \sum_{h=e}^{m} {\binom{m-e}{h-e}} (h+1)(-n)^{h-e}$$

If we let j = h - e and apply the binomial theorem twice we obtain the formula stated above. (Notice that this implies Weinberg's formula for w(n, k) when e = 0.)

THEOREM 6.13. If $0 \le e \le m - 1$ and $H = \langle m \rangle$, then

$$f(H, e, n) = \binom{m-1}{e} \binom{m}{n}^e \left(1 - \frac{m}{n}\right)^{m-1-e}.$$

If $0 \le h = m - l \le m - 1$, then it follows from the proof of Theorem 6.3 that

$$\sum' p(F_m) = \binom{m-1}{l-1} m^{m-l},$$

where the sum is over all spanning forests F_m of H that have l components and h edges. Hence,

$$\begin{aligned} f(H, e, n) &= \sum_{h=e}^{m-1} (-1)^{e} {h \choose e} {m-1 \choose h} \left(-\frac{m}{n}\right)^{h} \\ &= {m-1 \choose e} {m \choose n}^{e} \sum_{h=e}^{m-1} {m-1-e \choose h-e} \left(-\frac{m}{n}\right)^{h-e} \\ &= {m-1 \choose e} {m \choose n}^{e} \left(1-\frac{m}{n}\right)^{m-1-e}. \end{aligned}$$

COROLLARY 6.13.1. If n labelled nodes are partitioned into c subsets the ith of which has m_i nodes then there are

$$n^{c-2} \prod_{i=1}^{c} {m_i - 1 \choose e_i} m^{e_i} (n - m_i)^{m_i - 1 - e_i}$$

trees T_n that contain e_i edges that join two nodes in the *i*th subset for i = 1, 2, ..., c.

This corollary was first proved by Na and Rapoport (1967) who used matrix methods; they used the formula to show that if a graph with n nodes

64 The Method of Inclusion and Exclusion

and n - 1 edges is constructed at random, the probability that the graph is connected is increased by a factor ranging between one or two if the nodes are partitioned into subsets and only edges joining nodes from different subsets are used. Moon (1968a) showed that their formula could be deduced from Theorem 6.1. Notice that if $e_1 = \cdots = e_c = 0$, then this is the same as Corollary 6.3.1. Weinberg's formula for W(n, k) and Theorem 3.3, for example, can also be derived from special cases of Corollary 6.13.1.

THEOREM 6.14. If $0 \le e \le 2s - 1$ and $H = \langle s, s \rangle$, then

$$f(H, e, n) = \left(\frac{s}{n}\right)^{e} \left(1 - \frac{s}{n}\right)^{2s-e-2} \left\{ \binom{2s}{e} \left(1 - \frac{2s-e}{n}\right) - \binom{2(s-1)}{e-2} \right\}.$$

It follows from definition (6.6) and the proof of Theorem 6.4 that

$$f(\langle r, s \rangle, e, n) = \sum_{h=e}^{r+s-1} (-1)^{e} {h \choose e} \sum_{i+j=h} {r \choose i} {s \choose j} \left(-\frac{r}{n}\right)^{j-1} \left(-\frac{s}{n}\right)^{i-1} \left(\frac{rs}{n^{2}} - \frac{ij}{n^{2}}\right).$$

When r = s, the inner sum equals

$$\binom{2s}{h}\left(-\frac{s}{n}\right)^{h}-\binom{2(s-1)}{h-2}\left(-\frac{s}{n}\right)^{h}$$

and the remaining sum can be evaluated by using the binomial theorem.

6.6. Miscellaneous Results. A wheel W_{n+1} where $n \ge 3$ consists of a cycle of length *n* each node of which is joined to an (n + 1)st node; a ladder L_{2m} consists of two paths of length m - 1 such that corresponding nodes in the two paths are joined; the Möbius ladder M_{2r} where $r \ge 2$ consists of a cycle of length 2r in which diagonally opposite nodes are joined by an edge. Sedláček (1968, 1969, 1970) has shown that

$$c(W_{n+1}) = \left(\frac{3+\sqrt{5}}{2}\right)^n + \left(\frac{3-\sqrt{5}}{2}\right)^n - 2,$$

$$c(L_{2m}) = \frac{1}{2\sqrt{3}} \left\{ (2+\sqrt{3})^m - (2-\sqrt{3})^m \right\},$$

and

$$c(M_{2r}) = \frac{r}{2} \{ (2 + \sqrt{3})^r + (2 - \sqrt{3})^r + 2 \}$$

Let A_n denote the set of all positive integers q for which there exists a graph G_n such that $c(G_n) = q$; for example,

and
$$A_1 = A_2 = \{1\}, \quad A_3 = \{1, 3\}, \quad A_4 = \{1, 3, 4, 8, 16\}, \\ A_5 = \{1, 3, 4, 5, 8, 9, 11, 12, 16, 20, 21, 24, 40, 45, 75, 125\}.$$

Sedláček (1966) determined the nine largest elements of A_n for $n \ge 8$; in (1969) he showed that $|A_n| \ge \frac{1}{2}(n^2 - 3n + 4)$ and G. Baron presented a sharper bound for $|A_n|$ at the 1969 Oberwolfach Conference on Graph Theory. They also consider analogous problems for regular graphs.

Dambit (1965) and Sedláček (1966) have shown that a planer graph and its dual have the same number of spanning trees, assuming they both are connected and have no loops.

PROBLEMS ON RANDOM TREES

7.1. Random Mapping Functions. Let f denote a function that maps $\{1, 2, ..., n\}$ into $\{1, 2, ..., n\}$; we have seen that each such function determines a directed graph D = D(f) on n nodes in which an arc goes from i to j if and only if f(i) = j. In this section we shall use some of the earlier results to study the distribution of some parameters associated with such functions; Harris (1960) and Riordan (1962) give additional material and references on such problems.

In what follows we shall need to approximate various sums by integrals; we shall omit most of the details. Most of the estimates used are based on the fact that if 0 < t < 1, then

$$e^{-t/(1-t)} < 1 - t < e^{-t}.$$

It follows from this that if $1 \le k \le n$, then

$$\exp\left\{-\frac{k^2}{2(n+1-k)}\right\} \leq \frac{(n)_k}{n^k} \leq \exp\left\{-\frac{1}{n}\binom{k}{2}\right\};$$

in particular, if $k = o(n^{2/3})$ then

(7.1)
$$\frac{(n)_k}{n^k} = e^{-k^2/2n}(1+o(1))$$

Katz (1955) and Rényi (1959b) proved the following result (sometimes we shall say f has a certain property when we really mean the graph D(f) has the property).

THEOREM 7.1. If C(n) denotes the number of connected mapping functions f, then

$$\lim_{n\to\infty} C(n)/n^{n-1/2} = (\pi/2)^{1/2}.$$

We saw in Theorem 3.3 that there are $D(n, k) = (n)_k n^{n-k-1}$ connected functions f whose graph has a cycle of length k; hence,

$$C(n) = n^{n-1} \sum_{k=1}^{n} \frac{(n)_k}{n^k}$$

If we use the above inequalities and approximate the sum by an integral, we find that

$$\lim_{n\to\infty} C(n)/n^{n-1/2} = \int_0^\infty e^{-u^2/2} \, du = (\pi/2)^{1/2}$$

COROLLARY 7.1.1. The probability that a random mapping function f is connected is asymptotic to $(\pi/2n)^{1/2}$ as $n \to \infty$.

Notice that the limit of $C(n)/n^{n-1/2}$ is not changed if we omit the first one or two terms in the sum; hence, if we only consider functions f such that $f(i) \neq i$, the probability that D(f) is connected is asymptotic to

$$\{C(n)/n^{n-1/2}\}\cdot\{n^{n-1/2}/(n-1)^n\}\sim e(\pi/2(n-1))^{1/2}.$$

Katz gives a table of these probabilities for selected values of n up to 100.

COROLLARY 7.1.2. The number of connected (undirected) graphs with n labelled nodes and n edges is asymptotic to $(\pi/8n)^{1/2}n^n$, as $n \to \infty$.

Let γ_n denote the length of the cycle in the graph of a connected mapping function f. Since

$$\sum_{k=1}^{n} k(n)_{k}/n^{k} = \sum_{k=1}^{n} (n)_{k}/n^{k-1} - \sum_{k=1}^{n} (n)_{k+1}/n^{k} = n,$$

it follows that the expected value $E(\gamma_n)$ of γ_n satisfies the relation

$$E(\gamma_n) = \frac{n^{n-1}}{C(n)} \sum_{k=1}^n k(n)_k / n^k = n^n / C(n) \sim (2n/\pi)^{1/2}$$

More generally, if x is any positive constant and $P\{E\}$ denotes the probability of the event E, then we find that

$$\lim_{n \to \infty} P\{\gamma_n/n^{1/2} < x\} = (2/\pi)^{1/2} \int_0^x e^{-u^2/2} \, du$$
$$= (2\pi)^{-1/2} \int_{-x}^{+x} e^{-u^2/2} \, du$$

This implies the following result due to Rényi (1959b).

66

THEOREM 7.2. The distribution of $\gamma_n/n^{1/2}$ approaches, as $n \to \infty$, the distribution of the absolute value of a random variable that has a normal distribution with zero mean and unit variance.

Let δ_n denote the number of arcs that belong to cycles in the graph of a (not necessarily connected) mapping function f. The following result is due to Rubin and Sitgreaves (1954); see also Dénes (1967).

THEOREM 7.3. There are
$$k(n)_k n^{n-k-1}$$
 functions f such that $\delta_n = k$.

Consider one of the C(n + 1, k) rooted directed trees in which the (n + 1)st node is the root and has k arcs directed towards it. If we remove the root, then the k nodes originally joined to the root can be arranged on (directed) cycles in k! ways. Hence, appealing to Theorem 3.2, the number of functions f such that $\delta_n = k$ is equal to

$$k! C(n + 1, k) = k! \binom{n-1}{k-1} n^{n-k} = k(n)_k n^{n-k-1};$$

this also follows from the result of Blakely (1964) described in §3.5.

It follows from Theorem 7.3 that

$$\lim_{n \to \infty} E(\delta_n)/n^{1/2} = \lim_{n \to \infty} n^{-3/2} \sum_{k=1}^n k^2(n)_k/n^k = \int_0^\infty u^2 e^{-u^2/2} \, du = (\pi/2)^{1/2}$$

and

$$\lim_{n\to\infty} E(\delta_n^2)/n = \lim_{n\to\infty} n^{-2} \sum_{k=1}^n k^3(n)_k/n^k = \int_0^\infty u^3 e^{-u^2/2} \, du = 2,$$

so

$$E(\delta_n) \sim (\pi n/2)^{1/2}$$
 and $\sigma^2(\delta_n) \sim (2 - \pi/2)n$.

THEOREM 7.4. If x is any positive constant, then

$$\lim_{n\to\infty} P\{\delta_n/n^{1/2} < x\} = 1 - e^{-x^{2/2}}.$$

This follows from Theorem 7.3 and the fact that

$$\int_{x}^{\infty} u e^{-u^{2}/2} \, du = e^{-x^{2}/2}.$$

Rubin and Sitgreaves (1954) and Harris (1960) show that the distribution of δ_n is the same as the distribution of the number of nodes that can be reached along a directed path from a given node in the graph of a random mapping function f. Göbel (1963) has studied the distribution of the number $n - \delta_n$ of nodes that don't belong to cycles in the graph of a random mapping function f with the property that $f(i) \neq i$ for all i (it was in the course of doing this that he proved a result equivalent to Theorem 3.3); he also showed that the kth factorial moment of the number of cycles of length $i (\geq 2)$ in the graph of such a function tends to i^{-k} as $n \to \infty$.

The proof of the next result uses properties of the signless Stirling numbers c(m, t) of the first kind; they may be defined (see, for example, Riordan (1958; p. 71)) by the identity

(7.2)
$$C_m(x) = x(x+1)\cdots(x+m-1) = \sum_{k=1}^{m} c(m,k)x^k,$$

for
$$m = 1, 2, \ldots$$
 Since $C_m(x) = (x + m - 1)C_{m-1}(x)$, it follows that

$$c(m, k) = c(m - 1, k - 1) + (m - 1)c(m - 1, k)$$

This recurrence relation can be used to show by induction that there are c(m, k) permutations of *m* objects that consist of *k* cycles (to establish this same recurrence relation for the number of such permutations, consider separately the cases when the *n*th object does or does not belong to a unit cycle). We can now prove the following result given by Kruskal (1954); the derivation we give resembles the derivation given by Riordan (1962).

THEOREM 7.5. If τ_n denotes the number of components in the graph of a random mapping function f, then

$$E(\tau_n) = \sum_{k=1}^n \frac{1}{k} \frac{(n)_k}{n^k}.$$

There are $\binom{n-1}{m-1}n^{n-m}c(m,k)$ mapping functions f whose graph has m

edges belonging to $\tau_n = k$ cycles; this follows from a slight modification of the argument used to prove Theorem 7.4 if we use the combinatorial interpretation of the numbers c(m, k). Consequently,

$$E(\tau_n) = \sum_{k=1}^n k P\{\tau_n = k\} = \sum_{k=1}^n k \sum_{m=k}^n \binom{n-1}{m-1} n^{-m} c(m,k)$$
$$= \sum_{m=1}^n \binom{n-1}{m-1} n^{-m} \sum_{k=1}^m k c(m,k).$$

If we differentiate both sides of equation (7.2) and then set x = 1, we find that the inner sum equals $m! (1 + 1/2 + \cdots + 1/m)$. Hence,

$$E(\tau_n) = \sum_{m=1}^n m \frac{(n)_m}{n^{m+1}} \sum_{k=1}^m \frac{1}{k}$$
$$= \sum_{k=1}^n \frac{1}{k} \sum_{m=k}^n m \frac{(n)_m}{n^{m+1}}.$$

The required formula now follows from the fact that the inner sum is equal to

$$\sum_{m=k}^{n} (n + m - n)(n)_m / n^{m+1} = \sum_{m=k}^{n} (n)_m / n^m - \sum_{m=k}^{n} (n)_{m+1} / n^{m+1}$$
$$= (n)_k / n^k.$$

COROLLARY 7.5.1. $\lim_{n\to\infty} E(\tau_n)/\frac{1}{2}\log n = 1$.

If $k/n^{1/2} \to 0$, then $(n)_k/n^k \to 1$; if $k/n^{1/2} \to \infty$, then $(n)_k/n^k \to 0$. Hence, $E(\tau_n)$ is approximately equal to

$$\sum_{\leq n^{1/2}} \frac{1}{k} \sim \log\left(n^{1/2}\right)$$

when n is large.

Kruskal (1954) established Theorem 7.5 by solving a differential equation for a certain generating function; he obtained an integral formula for $E(\tau_n)$ from which he deduced that

$$E(\tau_n) = \frac{1}{2}\log n + \frac{1}{2}(\log 2 + C) + o(1)$$

where $C = 0.5772 \cdots$ is Euler's constant. (Recall that if f is a random permutation, then the expected number of cycles, or components, is $\log n + C + o(1)$.) It is not difficult to write expressions for the higher factorial moments of the distribution of τ_n . Austin, Fagen, Penney, and Riordan (1959) have considered the problem of determining the expected number of components in an undirected graph with a given number of nodes and edges.

7.2. The Degrees of the Nodes in Random Trees. If d(x) denotes the degree of node x in a random tree T_n , then it follows from Theorem 3.2 that

(7.3)
$$P\{d(x) = k\} = \binom{n-2}{k-1} \left(\frac{1}{n}\right)^{k-1} \left(1 - \frac{1}{n}\right)^{n-k-1},$$
for $k = 1, 2, ..., n-1$.

Consequently, d(x) (or rather d(x) + 1) has a binomial distribution and the mean and variance of d(x) are given by the formulas

E(d(x)) = 2(1 - 1/n) and $\sigma^2(d(x)) = (1 - 1/n)(1 - 2/n)$.

The distribution can be approximated by the Poisson distribution when n is large. In this section we shall show that the maximum degree $D = D(T_n)$ of the nodes of the tree T_n is approximately equal to $\log n/\log \log n$ for most trees T_n when n is large, and we shall consider the distribution of the number X = X(k, n) of nodes of degree k in a random tree T_n .

The following lemmas are quite straightforward consequences of the inequalities $(k/e)^k < k! < k^k$ and $t < -\log(1-t) < t/(1-t)$ where 0 < t < 1.

Lемма 7.1. If

$$k = \left[\frac{(1+\epsilon)\log n}{\log\log n}\right],$$

then $n/k! < n^{-\epsilon + o(1)}$ as $n \to \infty$, for any positive constant ϵ .

LEMMA 7.2. If

$$k = \left[\frac{(1-\epsilon)\log n}{\log\log n}\right],$$

then $n/k! > n^{\epsilon + o(1)}$ as $n \to \infty$, for any positive constant ϵ .

LEMMA 7.3. If $k = \lfloor \log n \rfloor$, then $n/k! < n^2 \log n/n^{\log \log n}$ for all sufficiently large values of n.

We now show that

(7.4) $P\{D > k\} \le n/k!;$

this and Lemma 7.1 imply that if ϵ is any positive constant, then

(7.5) $D \le (1 + \epsilon) \log n / \log \log n$

for almost all trees T_n , that is, for all but a fraction that tends to zero as $n \to \infty$.

It follows from (7.3) that

$$P\{d(x) = k\} = \frac{(1 - 1/n)^n}{(k - 1)!} \cdot \frac{n^2}{(n - 1)^2} \cdot \frac{(n - 2)_{k-1}}{(n - 1)^{k-1}} < \frac{e^{-1}}{(k - 1)!}, \quad \text{if } k \ge 3$$

(the last two expressions are asymptotically equal if $k = o(n^{1/2})$); therefore,

$$P\{d(x) > k\} < e^{-1}\left\{\frac{1}{k!} + \frac{1}{(k+1)!} + \cdots\right\} < \frac{e^{-1}}{k!}$$
$$\times \left\{1 + \frac{1}{k+1} + \frac{1}{(k+1)^2} + \cdots\right\} = \frac{e^{-1}}{k!}(1+1/k) < 1/k!, \quad \text{if } k \ge 2.$$

Inequality (7.4) now follows upon applying Boole's inequality

$$P\{\cup E_i\} \leq \sum P\{E_i\}$$

(the result is obviously true when k = 1). Next we show that

(7.6) $P\{D \le k\} < cn^{1/2} \exp(-n/e \cdot k!)$

for some positive constant c; this and Lemma 7.2 imply that if ϵ is any positive constant, then

 $D > (1 - \epsilon) \log n / \log \log n$

(7.7)

for almost all trees T_{n} .

If t(n, k) denotes the number of trees T_n such that $D(T_n) \le k$, then it follows from Theorem 3.1 that

t(n,k) = (n-2)!

× the coefficient of z^{n-2} in $\left\{1 + z + \frac{z^2}{2!} + \cdots + \frac{z^{k-1}}{(k-1)!}\right\}^n$;

hence,

$$t(n, k) < (n - 2)! \{1 + 1 + 1/2! + \dots + 1/(k - 1)!\}^n < (n - 2)! \{e - 1/k!\}^n < cn^{n - 3/2} \{1 - 1/e \cdot k!\}^n < cn^{n - 3/2} \cdot \exp(-n/e \cdot k!),$$

for some constant c, by Stirling's formula. If we divide this inequality by n^{n-2} , the total number of trees T_n , we obtain inequality (7.6). Moon (1968b) used these inequalities to prove the following result.

THEOREM 7.6. If E(D) denotes the expected value of the maximum degree of the nodes of a random tree T_n , then

$$E(D) \sim \frac{\log n}{\log \log n}, \quad as \ n \to \infty.$$

If ϵ is any positive constant, let

$$k_1 = \left[(1 + \epsilon) \frac{\log n}{\log \log n} \right]$$
 and $k_2 = [\log n]$.

Since

$$E(D) = \sum_{k=1}^{n-1} P\{D = k\} \le k_1 P\{D \le k_1\} + k_2 P\{D > k_1\} + (n-1)P\{D > k_2\},$$

it follows from (7.4) and Lemmas 7.1 and 7.3 that

$$E(D) \le (1 + \epsilon) \log n / \log \log n + (\log n) n^{-\epsilon + o(1)} + n^3 \log n / n^{\log \log n}$$

= (1 + \epsilon + o(1)) \log n / \log \log n, \quad \text{as } n \rightarrow \infty.

Furthermore,

$$E(D) \ge (1 - \epsilon) \frac{\log n}{\log \log n} P\left\{D > (1 - \epsilon) \frac{\log n}{\log \log n}\right\}$$
$$\ge (1 - \epsilon - o(1)) \frac{\log n}{\log \log n}, \quad \text{as } n \to \infty,$$

by inequality (7.7). These two inequalities suffice to prove the theorem because ϵ can be arbitrarily small.

If sharper inequalities for n/k! are used, then it can be shown that

$$(1-\epsilon)g(n) < D(T_n) - \frac{\log n}{\log \log n} < (1+\epsilon)g(n),$$

where

and

$$g(n) = (\log n)(\log \log \log n)(\log \log n)^{-2},$$

for almost all trees T_n and each positive constant ϵ .

Rényi (1959a) proved the case k = 1 of the following result; Meir and Moon (1968) stated the general formula.

THEOREM 7.7. If X = X(n, k) denotes the number of nodes of degree k in a random tree T_n and $p^{-1} = e \cdot (k - 1)!$, then

 $E(X) \sim np$

$$\sigma^{2}(X) \sim np(1-p) - np^{2}(k-2)^{2}$$

for each fixed value of k as $n \rightarrow \infty$.

If k is some fixed positive integer, let the variable x_i equal one if the *i*th node of a random tree T_n has degree k, and zero otherwise. Then

$$x_1 + x_2 + \cdots + x_n = X,$$

the number of nodes of degree k in T_n . It follows from equation (7.3) that

$$E(x_i) = E(x_i^2) = \frac{(1-1/n)^{n-2}}{(k-1)!} \cdot \frac{(n-1)_k}{(n-1)^k}$$
$$= p\{1-(k^2-k-3)/2n\} + 0(1/n^2)$$

and

$$\sigma^{2}(x_{i}) = E(x_{i}^{2}) - E^{2}(x_{i})$$

= $p(1 - p) - p(1 - 2p)(k^{2} - k - 3)/2n + O(1/n^{2});$

furthermore, it follows from Theorem 3.1 that

$$E(x_{i}x_{j}) = \frac{(1-2/n)^{n-2}}{(k-1)!^{2}} \cdot \frac{(n-2)_{2(k-1)}}{(n-2)^{2(k-1)}}$$
$$= p^{2}\{1 - (2k^{2} - 5k + 1)/n\} + O(1/n^{2})$$

and

Cov $(x_i, x_j) = E(x_i x_j) - E(x_i)E(x_j) = -p^2(k-2)^2/n + 0(1/n^2),$ for $1 \le i < j \le n$. Consequently,

$$E(X) = \sum_{i} E(x_{i}) = np - p(k^{2} - k - 3)/2 + O(1/n)$$

and

$$\sigma^{2}(X) = \sum_{i} \sigma^{2}(x_{i}) + 2 \sum_{i < j} \text{Cov}(x_{i}, x_{j})$$
$$= np(1 - p) - np^{2}(k - 2)^{2} + 0(1)$$

The distribution of $(X - \mu)/\sigma$, where $\mu = np$ and $\sigma^2 = np(1 - p) - p$ $np^{2}(k-2)^{2}$, tends to the normal distribution with zero mean and unit variance as $n \to \infty$. This was proved by Rényi (1959a) when k = 1 and by Meir and Moon (1968) when k = 2: the general result follows from the special case of a theorem proved by Sevast'vanov and Chistyakov (1964). (It is not difficult to show, using Theorem 3.1, that the hth factorial moment of X(n, k) tends to $(n)_k p^k$, the *h*th factorial moment of the binomial distribution, as $n \to \infty$. This is not enough, however, to show that the standardized distribution of X tends to the binomial distribution and hence to the normal distribution; the higher terms cannot be neglected in calculating the central moments. Notice that $\sigma^2(X)$ is asymptotic to what it would be if the variables x_1, x_2, \ldots, x_n were independent only when k = 2.

Theorem 3.5 states that the number R(n, k) of trees T_n for which X(n, 1) = k is given by the formula $R(n, k) = (n)_{n-k}S(n-2, n-k)$; it follows from equation (3.7) that

$$\sum_{k=2}^{n-1} R(n,k) \frac{(x)_{n-k}}{(n)_{n-k}} = x^{n-2}$$

Rénvi uses this relation to show that the characteristic function of $(X - \mu)/\sigma$ tends to the characteristic function of the normal distribution, that is,

$$\lim_{n\to\infty}\sum_{k=2}^{n-1}\frac{R(n,k)}{n^{n-2}}\exp\left\{it(k-\mu)/\sigma\right\}=e^{-t^{2}/2},$$

for every real t; this suffices to show that the distribution of $(X - \mu)/\sigma$ is asymptotically normal. (See also Weiss (1958) and Rényi (1962, 1966).)

If $0 \le k \le n-2$, let I(n, k) denote the number of trees T_n such that X(n, 2) = k. Such a tree can be formed by (1) choosing the k nodes whose degree is to be two, (2) constructing a tree T_{n-k} with no nodes of degree two, and (3) inserting the k nodes in the edges of the tree T_{n-k} . It follows, therefore, that

$$I(n, k) = \binom{n}{k}(n-2)_{k}I(n-k, 0),$$

and

$$n^{n-2} = \sum_{k=0}^{n-2} I(n,k) = \sum_{k=0}^{n-2} {n \choose k} (n-2)_k I(n-k,0).$$

If we let

$$f(n) = \frac{n^{n-2}}{(n-2)!}$$
 and $g(n) = \frac{I(n,0)}{(n-2)!}$

then this relation may be rewritten as

k = 0

$$f(n) = \sum_{k=0}^{n} \binom{n}{k} g(k),$$

for $n = 0, 1, \ldots$, if we assume that f(n) = g(n) = 0 when n = 0 or 1; if we invert this relation we find that

(7.8)
$$g(n) = \sum_{k=0}^{n} (-1)^{n-k} \binom{n}{k} f(k) = \sum_{k=2}^{n} (-1)^{n-k} \binom{n}{k} \frac{k^{k-2}}{(k-2)!}$$

Consequently.

$$I(n, k) = (n - 2)! \binom{n}{k} g(n - k)$$

= $(n - 2)! \binom{n}{k} \sum_{i=2}^{n-k} (-1)^{n-k-i} \binom{n-k}{i} \frac{i^{i-2}}{(i-2)!}$

(This formula can also be derived by the method of inclusion and exclusion.)

It follows from equation (7.8) or Theorem 3.1 that g(n) equals the coefficient of z^{n-2} in the expansion of $(e^z - z)^n$. Hence,

$$\frac{g(n)}{(e-1)^n} = \frac{1}{2\pi i} \int_C z \left\{ \frac{e^z - z}{z(e-1)} \right\}^n dz$$

where C is some contour about the origin, by Cauchy's integral formula. Meir and Moon (1968) use this fact to show that

$$\frac{g(n)}{(e-1)^n} \sim \{(e-1)/2\pi en\}^{1/2}$$

as $n \to \infty$. It now follows from Stirling's formula that

$$I(n, 0) \sim \left(1 - \frac{1}{e}\right)^{n+1/2} n^{n-2}.$$

(Notice that if we had assumed the variables x_1, x_2, \ldots, x_n were independent and that $P\{x_i = 1\} = 1/e$, we would have obtained the estimate $(1 - 1/e)^n n^{n-2}$ for I(n, 0).)

More generally, if $n - k \rightarrow \infty$, then

$$\frac{I(n,k)}{n^{n-2}} = \frac{(n-2)!}{n^{n-2}} \binom{n}{k} g(n-k)$$

$$\sim \frac{e^n (n-2)!}{(2\pi)^{1/2} n^{n-2}} \binom{n}{k} \left(\frac{1}{e}\right)^k \left(1-\frac{1}{e}\right)^{n-k} \left(\frac{e-1}{e(n-k)}\right)^{1/2}$$

$$\sim \binom{n}{k} \left(\frac{1}{e}\right)^k \left(1-\frac{1}{e}\right)^{n-k} \left(\frac{n(e-1)}{(n-k)e}\right)^{1/2}.$$

If α and β are constants such that

$$\frac{\alpha}{e}(n(e-1))^{1/2} < k - \frac{n}{e} < \frac{\beta}{e}(n(e-1))^{1/2},$$

then

$$\frac{n(e-1)}{(n-k)e} = 1 + \frac{k-n/e}{n-k} = 1 + 0(n^{-1/2}).$$

Hence, if $\sigma^2 = ne^{-1}(1 - e^{-1})$, then

$$P\{\alpha < (X - n/e)/\sigma < \beta\} = \sum' \frac{I(n,k)}{n^{n-2}} \sim \sum' \binom{n}{k} \left(\frac{1}{e}\right)^k \left(1 - \frac{1}{e}\right)^{n-k}$$

where the sums are over k such that $\alpha\sigma < k - n/e < \beta\sigma$. It now follows from the De Moivre-Laplace Theorem that the distribution of

$$(X(n,2) - n/e)/\sigma$$

tends to the normal distribution as $n \to \infty$.

7.3. The Distance between Nodes in Random Trees. If u and v are any two nodes in a tree T_n let $\delta_n = \delta(T_n; u, v)$ denote the number of nodes in the unique path joining u and v; the distance $d(u, v) = d(T_n; u, v)$ between u and v is the number of edges in this path so that $d(u, v) = \delta_n - 1$. In this section we consider some problems related to the distribution of the distance between nodes in a random tree T_n . The following result is due to Meir and Moon (1970a).

THEOREM 7.8. If $2 \le k \le n$, then

$$P\{\delta_n = k\} = \frac{k}{n-1} \cdot \frac{(n)_k}{n^k}$$

There are $(n-2)_{k-2}$ ways to construct a path from u to v that passes through k-2 of the remaining n-2 nodes and, by Theorem 6.1, there are kn^{n-k-1} trees T_n that contain any given path of k nodes. Hence, there are

$$(n-2)_{k-2}kn^{n-k-1} = kn^{n-k-2}(n)_k/(n-1)$$

Problems on Random Trees 77

trees T_n such that $\delta(T_n; u, v) = k$. If we divide this expression by n^{n-2} , the total number of trees T_n , we obtain the above formula for the probability that $\delta_n = k$.

It follows from Theorem 7.8 that $P\{\delta_n = 2\} = 2/n$ and

$$P\{\delta_n = k+1\} = \frac{k+1}{k} \cdot \frac{n-k}{n} P\{\delta_n = k\}, \quad \text{for } k = 2, 3, \dots, n-1.$$

It can be shown that

$$\max_{k} P\{\delta_n = k\} = (1 + o(1))(en)^{-1/2};$$

if $t = [n^{1/2}]$, the maximum occurs when k = t or t + 1 according as $t(t + 1) \ge n$ or $t(t + 1) \le n$.

If we compare Theorems 7.3 and 7.8 we see that when n is large the probability that there are k nodes in the path joining u and v is very close to the probability that there are k arcs that belong to cycles in the graph of a random mapping function f. The proof of the following result involves the same arguments as were outlined after Theorem 7.3 (see Meir and Moon for the missing details).

THEOREM 7.9. The mean and variance of δ_n satisfy the relations

$$E(\delta_n) \sim (\frac{1}{2}\pi n)^{1/2}$$

and

$$\sigma^2(\delta_n) \sim (2 - \pi/2)n$$

as $n \rightarrow \infty$; furthermore, if x is any positive constant, then

 $\lim_{n\to\infty} P\{\delta_n/n^{1/2} < x\} = 1 - e^{-x^{2/2}}.$

Mr. J. Hubert calculated the entries in Table 3.

TABLE 3

n	$E(\delta_n)$	$E(\delta_n^2)$	n	$E(\delta_n)$	$E(\delta_n^2)$
2	2	4	12	4.312	21.688
3	2.333	5.667	14	4.642	25.358
4	2.625	7.375	16	4.951	29.049
5	2.888	9.112	18	5.243	32.757
6	3.130	10.870	20	5.520	36.480
7	3.354	12.646	25	6.159	45.841
8	3.566	14.434	50	8.697	93.303
9	3.766	16.234	100	12.323	189.677
10	3.956	18.044	150	15.119	286.881

Problems on Random Trees 79

If $\lambda_n = \lambda(T_n, k)$ denotes the number of paths of length k - 1 in a tree T_n , then it can be shown that

 $E(\lambda_n) = \frac{1}{2}kn\frac{(n)_k}{n^k}$

and

$$\sigma^2(\lambda_n) \sim nk(k-1)^2(k-2)/24$$

for each fixed value of k as $n \to \infty$. The argument used in this section can also be modified to show that the expected number of inversions in a random tree T_n (see §4.5) is equal to

$$\frac{1}{2}\sum_{k=1}^{n}k^{2}(n)_{k}/n^{k}-n+\frac{1}{2}\sim(\pi/8)^{1/2}n^{3/2}.$$

7.4. Trees with Given Height and Diameter. If the tree T_n is rooted at a given node u, then the height $h_n = h(T_n, u)$ of T_n (with respect to u) is the maximum of d(u, v) taken over all nodes v of T_n ; let $t_n(k)$ denote the number of trees T_n such that $h(T_n, u) \le k$ (notice that $t_n(k) = 0$ unless $1 \le k \le n - 1$, except that $t_1(0) = 1$). If

$$G_k = G_k(x) = \sum_{n=1}^{\infty} nt_n(k) \frac{x^n}{n!}$$

denotes the generating function for the number of rooted trees with height at most k, then $G_k^l/l!$ is the generating function for forests of l rooted trees each of whose height is at most k; this follows by the same argument as was used in §4.1. If we join the roots of these l trees to a new node we obtain, in effect, a rooted tree with one additional node whose height is at most k + 1. It follows, therefore, that $G_0 = x$ and

(7.9)
$$G_{k+1} = x + xG_k + xG_k^2/2! + \cdots = x \exp G_k$$

for k = 0, 1, ...; this relation was derived by Riordan (1960) and Rényi and Szekeres (1967). (Harris and Schoenfeld (1967, 1968, 1970) have considered, among other things, a problem equivalent to determining the asymptotic expansion of the coefficients in $G_2 = x \exp xe^x$.) If

$$H_k = H_k(x) = \sum_{n=1}^{\infty} nh_n(k) \frac{x^n}{n!},$$

where $h_n(k) = t_n(k) - t_n(k-1)$, denotes the generating function for the number of rooted trees of height k, then $H_0 = x$ and

$$H_k(x) = G_k(x) - G_{k-1}(x)$$

for k = 1, 2, ... (Riordan gives a table of the numbers $h_n(k)$ for $1 \le k < n \le 10$). Rényi and Szekeres use (7.9) and the fact that

$$\frac{h_n(k)}{(n-1)!} = \frac{1}{2\pi i} \int_C \frac{G_k(z) - G_{k-1}(z)}{z^{n+1}} \, dz$$

where C is a contour about the origin, to determine the asymptotic distribution of the numbers $h_n(k)$ for large n and k. Their argument is quite complicated; they show, among other things, that

$$E(h_n) \sim (2\pi n)^{1/2}$$
 and $\sigma^2(h_n) \sim \frac{1}{3}\pi(\pi - 3)n$,

as $n \to \infty$. Notice that $E(\delta_n) \sim \frac{1}{2}E(h_n)$ as $n \to \infty$.

The diameter $d(T_n)$ of a tree T_n is the greatest distance between any two nodes of T_n , that is,

$$d(T_n) = \max \{ d(u, v) : u, v \in T_n \} = \max \{ h(T_n, u) : u \in T_n \};$$

if $n \ge 3$, then $2 \le d(T_n) \le n - 1$ and $h(T_n) \le d(T_n) \le 2h(T_n)$. Let $r_n(k)$ denote the number of trees T_n such that $d(T_n) = k$; we now derive an expression for the generating function

$$D_k = D_k(x) = \sum_{n=1}^{\infty} r_n(k) \frac{x^n}{n!}$$

Any tree with odd diameter 2h + 1 can be formed by joining the roots of two rooted trees each of height h (such trees are said to be *bicentred*; see König (1936; chapter 5)). It follows, therefore, that

$$D_{2h+1}(x) = \frac{1}{2}H_h^2(x).$$

Any tree with even diameter 2h can be formed by identifying the roots of two or more rooted trees of height at most h if at least two of these trees have height h (such trees are said to be *centred*). In fact, every rooted tree of height h has diameter 2h except for those in which the root is incident with only one edge leading to nodes whose distance from the root is h; the generating function for these exceptions is $G_{h-1} cdot H_{h-1}$. It follows, therefore, that

$$D_{2h}(x) = H_h(x) - G_{h-1}(x) \cdot H_{h-1}(x)$$

These relations for $D_k(x)$ were derived by Riordan; he gives a table of the numbers $r_n(k)$ for $2 \le k < n \le 10$. The asymptotic distribution of these numbers apparently has not been determined.

7.5. The First Two Moments of the Complexity of a Graph. We mentioned earlier that in certain physical problems there is a correspondence between the terms in the nth successive approximation to certain functions

and graphs with certain properties. There is at least one case where the actual value of the terms has a graph-theoretical interpretation.

The coefficients in the expansion of various thermodynamic quantities of a gas can be expressed as a sum of integrals, called cluster integrals, which correspond to graphs with a given number of nodes and edges; there is a factor in the integrand, representing the intermolecular potential function, corresponding to each edge of the graph. Uhlenbeck and Ford (1962; see also 1963) show that if the intermolecular potential is a gaussian function of the type $f(r) = -e^{-\alpha r^2}$, then the cluster integral corresponding to the graph G can be expressed in terms of the number c(G) of spanning trees of G (the number c(G) is sometimes called the *complexity* of the graph G in physical contexts; see also Temperley (1964)).

It would be of some interest to know the distribution of the number c = c(n, e) of spanning trees of graphs with *n* nodes and *e* edges; Uhlenbeck and Ford (1962) give numerical data which suggests that the distribution of *c* tends to the normal distribution as *n* increases if *e* is near $\frac{1}{2}N = \frac{1}{4}n(n-1)$. It seems, however, that formulas for only the first two moments are known in general; we now derive formulas for E(c) and

 $E(c^2)$ where the expectations are taken over the $\binom{N}{e}$ graphs with *n* nodes and *e* edges.

THEOREM 7.10. If $n - 1 \le e \le N$, then

$$E(c) = n^{n-2} \frac{(e)_{n-1}}{(N)_{n-1}} \cdot$$

Each of the n^{n-2} trees T_n has n-1 edges; hence, the number of graphs with n nodes and e edges containing any such tree is the number of ways of selecting e - (n-1) of the N - (n-1) pairs of nodes not already joined by an edge. Therefore,

$$E(c) = n^{n-2} \binom{N-(n-1)}{e-(n-1)} \cdot \binom{N}{e}^{-1} = n^{n-2} \frac{(e)_{n-1}}{(N)_{n-1}}$$

THEOREM 7.11. If $n - 1 \le e \le N$, then

$$E(c^{2}) = \sum_{m=0}^{n-1} T_{m}(n) \sum_{j=0}^{m} (-1)^{m-j} {m \choose j} \frac{(e)_{2(n-1)-j}}{(N)_{2(n-1)-j}}$$

where

$$T_m(n) = n^{2(n-m-2)}(n-1)_m \sum_{t=0}^m \binom{n-t}{m-t} \frac{n^t}{t!}.$$

We first determine an expression for the number $T_m(n)$ of ordered pairs of trees with *n* nodes that have at least $m (\leq n - 1)$ edges in common (each such pair of trees is counted separately for each set of m edges they have in common). If two trees have m edges in common then these m edges and the n nodes determine a forest of l = n - m subtrees. It follows from Theorem 6.1 and the derivation of Theorem 4.1 that

$$T_m(n) = \frac{n^{2(l-2)}}{l!} \sum {\binom{n}{j_1,\ldots,j_l}} j_1^{j_1-2} \cdots j_l^{j_l-2} \cdot (j_1 \cdots j_l)^2,$$

where the sum is over all compositions of n into l positive integers. If

$$U = U(x) = \sum_{j=1}^{\infty} \frac{j^j x^j}{j!}$$
 and $Y = Y(x) = \sum_{j=1}^{\infty} j^{j-1} \frac{x^j}{j!}$,

then U = x Y'; since $Y = xe^{Y}$ it follows that $U = Y(1 - Y)^{-1}$. If $B_{l}(n) = l! n^{-2(l-2)}T_{m}(n)$, then

$$\sum_{n=1}^{\infty} B_{l}(n) \frac{x^{n}}{n!} = U^{l} = Y^{l}(1 - Y)^{-l} = \sum_{t=0}^{\infty} {\binom{l+t-1}{t}} Y^{l+t};$$

but

$$Y^{l+t} = (l+t) \sum_{n=l+t}^{\infty} n^{n-l-t-1}(n)_{l+t} \frac{x^n}{n!},$$

by equation (4.2). Therefore,

$$T_{m}(n) = \frac{n^{2(l-2)}}{l!} B_{l}(m) = \frac{n^{2(l-2)}}{l!} \sum_{t=0}^{n-l} (l+t) \binom{l+t-1}{t} (n)_{l+t} n^{n-l-t-1}$$
$$= n^{2(n-m-1)} (n-1)_{m} \sum_{t=0}^{m} \binom{n-t}{m-t} \frac{n^{t}}{t!}.$$

If we apply the method of inclusion and exclusion, we find that there are

$$\sum_{j=0}^{n-1-m} (-1)^{j} \binom{m+j}{m} T_{m+j}(n)$$

ordered pairs of trees with n nodes that have exactly m edges in common. The probability that a graph with n nodes and e edges will contain a given pair of such trees is

$$\binom{N-2(n-1)+m}{e-2(n-1)+m} \cdot \binom{N}{e}^{-1} = (e)_{2(n-1)-m}/(N)_{2(n-1)-m}$$

It follows, therefore, that

$$E(c^{2}) = \sum_{m=0}^{n-1} \frac{(e)_{2(n-1)-m}}{(N)_{2(n-1)-m}} \sum_{j=0}^{n-1-m} (-1)^{j} \binom{m+j}{m} T_{m+j}(n)$$

=
$$\sum_{m=0}^{n-1} T_{m}(n) \sum_{j=0}^{m} (-1)^{m-j} \binom{m}{j} \frac{(e)_{2(n-1)-j}}{(N)_{2(n-1)-j}}.$$

COROLLARY 7.11.1. If $\lim_{n\to\infty} e/N = \gamma$, where $0 < \gamma < 1$, then

$$\lim_{n\to\infty}\frac{E(c^2)}{E^2(c)}=1.$$

Let $R_m(n)$ denote the inner sum in the formula for $E(c^2)$ so that

$$E(c^2) = \sum_{m=0}^{n-1} T_m(n) \cdot R_m(n)$$

If $\phi(n, e) = n^{2(n-2)}(e)_{2(n-1)}/(N)_{2(n-1)}$, then

$$\lim_{n \to \infty} \frac{T_m(n) \cdot R_m(n)}{\phi(n, e)} = \sum_{t=0}^m \frac{1}{t! (m-t)!} \cdot \sum_{j=0}^m (-1)^{m-j} {m \choose j} \gamma^{-j}$$
$$= \frac{2^m}{m!} \cdot \frac{(1-\gamma)^m}{\gamma^m}$$

for each fixed value of m; it follows therefore, from Tannery's theorem (see Bromwich (1931)) that

$$\lim_{n\to\infty}\frac{E(c^2)}{\phi(n,e)}=\exp 2(1-\gamma)/\gamma$$

The corollary now follows from Theorem 7.10 and inequality (7.1).

Theorems 7.10 and 7.11 were proved by Uhlenbeck and Ford (1962) and Moon (1964), respectively; Groeneveld (1965) has given another derivation of Theorem 7.11 that also applies to graphs in which several edges may join the same pair of nodes.

We remark that Erdös and Rényi (1960) have shown that if $e \sim \rho n^{(k-2)/(k-1)}$, then the distribution of the number of isolated trees with k nodes in a random graph with n nodes and e edges tends to the Poisson distribution with mean

$$\lambda = \frac{(2\rho)^{k-1}k^{k-2}}{k!}$$

as $n \rightarrow \infty$; Palásti (1961) has obtained an analogous result for bipartite trees.

7.6. Removing Edges from Random Trees. If some edges of a tree T_n are removed the graph remaining is a forest of disjoint subtrees of T_n ; let r denote the number of nodes in the subtree containing a given node x (say the *n*th node). In this section we shall determine the distribution of r under the assumptions that (1) the tree T_n is chosen at random from the set of n^{n-2} trees with n labelled nodes, and (2) the edges removed from T_n are chosen independently at random so that any given edge is removed with probability p = 1/2; in particular, we shall show that the mean E(r) and variance $\sigma^2(r)$ of r tend to 4 and 16, respectively, as n tends to infinity.

THEOREM 7.12. If $1 \le k \le n$, then

$$P\{r = k\} = (2n)^{1-n} \binom{n}{k} k^k (2n - k)^{n-k-1}.$$

If r = k, then there are $\binom{n-1}{k-1}k^{k-2}$ choices possible for the subtree T_k that contains node x and k-1 other nodes after a random selection of edges has been removed from a random tree T_n . If $1 \le k < n$, let j denote the number of edges in T_n that joined nodes of T_k to nodes not in T_k ; the probability that these edges were removed and the k-1 edges of T_k were left intact is $(1/2)^{j+k-1}$. There are $\binom{n-k-1}{j-1}k^j(n-k)^{n-k-j}$ trees T_n that contain a given tree T_k on k given nodes and such that j edges join nodes of T_k to nodes not in T_k ; this follows from Theorem 3.2 if we temporarily consider T_k as a special node y, construct a tree on node y and the remaining n-k nodes in which d(y) = j, and then replace the j edges incident with y by edges incident with one of the k nodes of T_k . It follows, therefore, that if $1 \le k < n$, then

$$P\{r=k\} = n \cdot (2n)^{1-n} \binom{n-1}{k-1} k^{k-1} \sum_{j=1}^{n-k} \binom{n-k-1}{j-1} k^{j-1} (2n-2k)^{n-k-j}$$
$$= (2n)^{1-n} \binom{n}{k} k^k (2n-k)^{n-k-1};$$

the formula is clearly valid when k = n also. Notice that

$$\lim_{n\to\infty} P\{r=k\} = (2\sqrt{e})^{-k} \frac{k^k}{k!}$$

for each fixed value of k.

We shall use some of the identities in Table 1 to simplify the expressions we obtain from Theorem 7.12 for E(r) and $E(r^2)$. If x = 0, y = n, p = 1, 4+c.t.t.

and q = -1, then it follows from the third identity in Table 1 that

$$A_n(0, n; 1, -1) = \sum_{k=0}^n \binom{n}{k} k^{k+1} (2n-k)^{n-k-1}$$

= $n^{-1} [\beta(0) + 2n]^n = n^{-1} \sum_{k=0}^n \binom{n}{k} k \cdot k! (2n)^{n-k}$
= $2(2n)^{n-1} \sum_{k=0}^n k(n)_k / (2n)^k.$

Furthermore,

$$[\beta(0;2)]^{k} = [\beta(0) + \beta(0)]^{k} = \sum_{t=0}^{k} {\binom{k}{t}} t \cdot t! (k-t) \cdot (k-t)!$$
$$= k! \sum_{t=0}^{k} t(k-t) = k! {\binom{k+1}{3}},$$

and

$$(\alpha + \gamma(0))^{k} = \sum_{t=0}^{k} {\binom{k}{t}} t^{2} \cdot t \, ! \, (k-t)! = \frac{1}{6} k! \, k(k+1)(2k+1);$$

it follows from the fourth identity in Table 1, after some simplification, that

$$A_n(0, n; 2, -1) = \sum_{k=0}^n \binom{n}{k} k^{k+2} (2n-k)^{n-k-1}$$

= $n^{-1} \{ (2n+\beta(0; 2))^n + (2n+\alpha+\gamma(0))^n \}$
= $(2n)^{n-1} \sum_{k=0}^n k^2 (k+1) \cdot (n)_k / (2n)^k.$

COROLLARY 7.12.1. $\lim_{n\to\infty} E(r) = 4$ and $\lim_{n\to\infty} \sigma^2(r) = 16$.

It follows from Theorem 7.12 and the identity for $A_n(0, n; 1, -1)$ that

$$E(r) = (2n)^{1-n} \sum_{k=0}^{n} {n \choose k} k^{k+1} (2n-k)^{n-k-1}$$
$$= 2 \sum_{k=0}^{n} k(n)_{k} / (2n)^{k};$$

therefore,

$$\lim_{n \to \infty} E(r) = 2 \sum_{k=0}^{\infty} k(1/2)^k = 4$$

by Tannery's Theorem (see Bromwich (1931)). Similarly,

$$E(r^{2}) = (2n)^{1-n} \sum_{k=0}^{n} {n \choose k} k^{k+2} (2n-k)^{n-k-1}$$
$$= \sum_{k=0}^{n} k^{2} (k+1) \cdot (n)_{k} / (2n)^{k}$$

and

$$\lim_{n\to\infty} E(r^2) = \sum_{k=0}^{\infty} k^2(k+1)(1/2)^k = 32;$$

consequently,

$$\lim_{n\to\infty}\sigma^2(r)=\lim_{n\to\infty}\left(E(r^2)-E^2(r)\right)=16$$

These results are due to Moon (1970a); the formula for E(r) can also be derived from Theorem 7.8. More generally, if the probability of removing any given edge of T_n is p, where 0 , then it can be shownthat

$$P\{r = k\} = \frac{p}{1-p} \left(\frac{1-p}{n}\right)^{n-1} {n \choose k} k^k \left(\frac{n}{1-p} - k\right)^{n-k-1},$$
$$\lim_{n \to \infty} E(r) = p^{-2},$$

and

$$\lim_{n\to\infty}\sigma^2(r)=2(1-p)p^{-4}$$

Professor N. J. Pullman computed the following values of E(r) and $E(r^2)$ when p = 1/2.

TABLE 4

1	E(r)	<i>E</i> (<i>r</i> ²)	n	E(r)	<i>E</i> (<i>r</i> ²)
1	1	1	11	2.8918	12.478
2	1.5	2.5	12	2.9529	13.194
3	1.8333	4	13	3.0073	13.8592
4	2.0781	5.4062	14	3.0562	14.477
5	2.268	6.7	15	3.1004	15.0552
6	2.4207	7.8837	20	3.2698	17.445:
7	2.5468	8.9661	25	3.3846	19.237
8	2.6530	9.9573	50	3.6539	24.078
9	2.7439	10.8673	100	3.8148	27.482
0	2.8227	11.7050	200	3.9039	29.567

7.7. Climbing Random Trees. If the tree T_n where $n \ge 2$ is rooted at node x suppose we select some edge incident with x and proceed along it to node y; then we select some other edge yz incident with y and proceed to z. If we continue this process as long as possible, let $s = s(T_n)$ denote the number of edges traversed before we reach some endnode u (other than x, if x is an endnode). In this section we shall determine the mean E(s) and variance $\sigma^2(s)$ of s under the assumptions that (1) the tree T_n is chosen at random from the n^{n-2} trees T_n that are rooted at node x, and (2) whenever we reach a node q that isn't an endnode, the next edge is chosen at random from the edges incident with q that lead away from x; it will follow that $E(s) \rightarrow 2e - 1$ and $\sigma^2(s) \rightarrow 2e(e - 1)$ as $n \rightarrow \infty$. The different rooted trees T_4 are illustrated in Figure 12 along with their relative frequencies and the calculations showing that E(s) = 17/8 when n = 4.





If y is any node joined to the root x of a tree T_n , then y can be thought of as the root of the subtree T^* determined by those nodes z of T_n such that the unique path joining x and z contains the edge xy. Let $\rho(n, k)$ denote the probability that the subtree T^* of a random rooted tree T_n has k nodes.

LEMMA 7.4. If $1 \le k \le n - 1$, then

$$\rho(n,k) = \frac{1}{n^{n-2}} \binom{n-1}{k-1} k^{k-2} (n-k-1)^{n-k-1}.$$

The k nodes of T^* can be chosen in $\binom{n-1}{k}$ ways and, having chosen the nodes, T^* can be formed in k^{k-2} ways. If the root x has degree t in T_n , where $1 \le t \le n-k$, then by Theorem 3.2 there are

$$\binom{n-k-2}{t-2}(n-k-1)^{n-k-t}$$

ways to form a tree on the n - k nodes not in T^* . The node y in T^* that is joined to the root x can be chosen in k ways and this node y could have been any one of the t nodes joined to x. Hence,

$$\rho(n,k) = \frac{1}{n^{n-2}} \sum_{t=1}^{n-k} \frac{1}{t} \binom{n-1}{k} \binom{n-k-2}{t-2} k^{k-1} (n-k-1)^{n-k-t}$$
$$= \frac{k^{k-2}}{n^{n-2}} \binom{n-1}{k-1} \sum_{t=1}^{n-k} \binom{n-k}{t} (t-1)(n-k-1)^{n-k-t-1}.$$

The lemma now follows by applying the binomial theorem (twice) to replace the sum by $(n - k - 1)^{n-k-1}$.

THEOREM 7.13. If $n \ge 1$, then

$$E(s) = 2\left(\frac{n+1}{n}\right)^{n-2} - 1$$

and

$$E(s(s-1)) = 6\left(\frac{n+2}{n}\right)^{n-2} - 8\left(\frac{n+1}{n}\right)^{n-2} + 2.$$

COROLLARY 7.13.1. As $n \to \infty$, $E(s) \to 2e - 1$ and $\sigma^2(s) \to 2e(e - 1)$.

If $0 \le l \le n - 1$, let P(n, l) denote the probability that $s(T_n) = l$; we adopt the convention that P(n, 0) = 1 if n = 1 and zero otherwise.

Suppose we select one of the edges xy incident with the root x of a random tree T_n and proceed along it to y; then $s(T_n) = l$ if and only if $s(T^*) = l - 1$, where T^* is the subtree defined earlier. Hence, if $1 \le l \le n - 1$ then it follows from Lemma 7.4 that

$$P(n, l) = \sum_{k=1}^{n-1} \rho(n, k) \cdot P(k, l-1)$$

= $\frac{1}{n^{n-2}} \sum_{k=1}^{n-1} {n-1 \choose k-1} k^{k-2} (n-k-1)^{n-k-1} P(k, l-1).$

If $\mu(n) = E(s)$, then

$$\mu(n) = \sum_{l=1}^{n-1} lP(n, l)$$

= $\frac{1}{n^{n-2}} \sum_{k=1}^{n-1} {\binom{n-1}{k-1}} k^{k-2} (n-k-1)^{n-k-1} \{\mu(k)+1\}$

for n = 2, 3, ..., if we substitute the formula for P(n, l) and interchange the order of summation ($\mu(1) = 0$ by definition). We can now prove the

formula for $\mu(n)$ by induction. If we assume $\mu(k) + 1 = 2(1 + 1/k)^{k-2}$ and apply the second identity in Table 1 with x = 2, y = -1 and n and k replaced by n - 1 and k - 1, we find that

$$\mu(n) = \frac{2}{n^{n-2}} \sum_{l=1}^{n-1} \binom{n-1}{k-1} (k+1)^{k-2} (n-k-1)^{n-k-1}$$
$$= \frac{2}{n^{n-2}} \{-\frac{1}{2}n^{n-2} + (n+1)^{n-2}\} = 2\left(\frac{n+1}{n}\right)^{n-2} - 1$$

as required.

Similarly, if $\tau(n) = E(s(s-1))$ then

$$\tau(n) = \sum_{l=1}^{n-1} l(l-1)P(n,l)$$

= $\frac{1}{n^{n-2}} \sum_{k=1}^{n-1} {n-1 \choose k-1} k^{k-2}(n-k-1)^{n-k-1} \{\tau(k) + 2\mu(k)\}$

If we assume, as our induction hypothesis, that

$$\tau(k) + 2\mu(k) = 6\left(\frac{k+2}{k}\right)^{k-2} - 4\left(\frac{k+1}{k}\right)^{k-2}$$

and apply the second identity in Table 1 twice, we find that

$$\begin{aligned} \tau(n) &= \frac{1}{n^{n-2}} \sum_{k=1}^{n-1} \binom{n-1}{k-1} \{ 6(k+2)^{k-2} - 4(k+1)^{k-2} \} (n-k-1)^{n-k-1} \\ &= \frac{1}{n^{n-2}} \{ 6[-\frac{2}{3}(n+1)^{n-2} + (n+2)^{n-2}] - 4[-\frac{1}{2}n^{n-2} + (n+1)^{n-2}] \} \\ &= 6 \left(\frac{n+2}{n}\right)^{n-2} - 8 \left(\frac{n+1}{n}\right)^{n-2} + 2, \end{aligned}$$

as required. The corollary follows immediately from the theorem and the fact that $\sigma^2(s) = E(s(s-1)) + E(s) - E^2(s)$.

Theorem 7.13 can also be proved by expressing the generating functions of the numbers $\mu(n)$ and $\tau(n)$ in terms of the function $Y = \sum_{n=1}^{\infty} n^{n-1} x^n/n!$ and then applying formula (4.2) (see Moon (1970b)). It can be shown that if $1 \le l \le n-1$, then

$$P(n, l) = \frac{l}{n^{n-2}} \sum_{j=0}^{l-1} {\binom{l-1}{j}} (-1)^j (n-2-j)^{n-2}.$$

Thus

$$P_{l} = \lim_{n \to \infty} P(n, l) = l p^{2} q^{l-1}$$

for l = 0, 1, ..., where $p = 1 - q = e^{-1}$, and the distribution of $s(T_n) - 1$ tends to the negative binomial distribution of order two as $n \to \infty$.

If $1 \le t \le n - 1$ and $\mu(n, t)$ and $\tau(n, t)$ denote the expected value of s and s(s - 1) over the set of trees T_n in which the root x has degree t, then the preceding arguments can be extended to show that

$$\mu(n,t) = \frac{t+1}{t} \left(\frac{n}{n-1}\right)^{n-t-2}$$

and

$$\tau(n, t) = \frac{2}{t} \left\{ (t+2) \left(\frac{n+1}{n-1} \right)^{n-t-2} - (t+1) \left(\frac{n}{n-1} \right)^{n-t-2} \right\}.$$

As a partial verification, notice that

$$\sum_{t=1}^{n-1} P\{d(x) = t\}\mu(n, t) = \sum_{t=1}^{n-1} \binom{n-1}{t}(t+1)n^{-t}$$
$$= 2\left(\frac{n+1}{n}\right)^{n-1} - 1 = \mu(n),$$

by Theorem 3.2 and the binomial theorem.

D. A. Klarner pointed out, in a letter dated March, 1969, that there are $n(n-1)^{n-1}$ ways to select a tree T_n , choose a root node x, and then proceed along a path from x to some endnode; hence, the average number of ways of rooting a tree T_n and then proceeding from the root to some endnode is

$$\frac{n(n-1)^{n-1}}{n^{n-2}} \sim n^2/e.$$

Perhaps it should be emphasized that E(s) is not the same as the average distance between the root x and a node u given that u is an endnode. The second proof of Theorem 3.2 and the proof of Theorem 7.8 can be modified to show that if u is an endnode then the expected distance between x and u is

$$\frac{1}{n-1}\sum_{t=1}^{n-1}t^2\frac{(n-1)_t}{(n-1)^t}$$

if x and u are both endnodes the expected distance between them is

$$\frac{1}{n-2}\sum_{t=1}^{n-2}t(t+1)\,\frac{(n-2)_t}{(n-2)^t}$$

if $n \ge 3$. Both of these quantities are asymptotic to the expected distance between two arbitrary nodes in a random tree T_n as $n \to \infty$.

7.8. Cutting Down Random Trees. Suppose the tree T_n where $n \ge 2$ is rooted at a given node x. If we remove some edge e of T_n the tree falls into two subtrees one of which, T_k say, contains the root x; if $k \ge 2$ we can remove some edge of T_k and obtain an even smaller subtree containing x. If we repeat this process as long as possible, let $\lambda = \lambda(T_n)$ denote the number of edges removed before we obtain the subtree consisting of the root x itself. In this section we shall determine the mean $\mu(n)$ and variance $\sigma^2(n)$ of $\lambda(T_n)$ under the assumptions that (1) T_n is chosen at random from the n^{n-2} trees T_n that are rooted at node x, and (2) at each stage the edge removed is chosen at random from edges of the remaining subtree containing x; it will follow that $\mu(n) \sim (\frac{1}{2}\pi n)^{1/2}$ and $\sigma^2(n) \sim (2 - \frac{1}{2}\pi)n$ as $n \to \infty$. These and some related results are due to Meir and Moon (1970b). (The average values of $\lambda(T_n)$ for the different trees T_4 are indicated in Figure 13; it can be shown that if T_n is a path rooted at an endnode, for example, then $E(\lambda(T_n)) = 1 + 1/2 + \cdots + 1/(n - 1)$.)



THEOREM 7.14. If n > 2, then

$$\mu(n) = \sum_{j=1}^{n-1} \frac{j+1}{j} \cdot \frac{(n-1)_j}{n^j}.$$

COROLLARY 7.14.1. As $n \to \infty$,

$$\mu(n) = (\frac{1}{2}\pi n)^{1/2} + \frac{1}{2}\log n + O((\log n)^{1/2}).$$

If $0 \le l \le n - 1$, let P(n, l) denote the probability that $\lambda(T_n)$ equals l; we adopt the convention that P(n, 0) equals one if n = 1 and zero otherwise.

Suppose we remove one of the n-1 edges of a random tree T_n and obtain a subtree T_k containing the root x. There are $\binom{n-1}{k-1}$ possible

choices for the k - 1 nodes of T_k other than x and, having chosen these nodes, there are k^{k-2} possible trees T_k . There are $(n - k)^{n-k-2}$ trees that could be formed on the remaining n - k nodes and the removed edge could have joined any of the k nodes of T_k to any of the remaining n - k nodes. Since $\lambda(T_n) = l$ if and only if $\lambda(T_k) = l - 1$, it follows that

(7.10)
$$P(n, l) = \frac{1}{(n-1)n^{n-2}} \sum_{k=l}^{n-1} {n-1 \choose k-1} P(k, l-1) k^{k-1} (n-k)^{n-k-1}$$

for $1 \leq l \leq n-1$.

If $\mu(n)$ denotes the expected value of $\lambda(T_n)$, then

(7.11)
$$\mu(n) = \sum_{l=1}^{n-1} lP(n, l)$$
$$= \frac{1}{(n-1)n^{n-2}} \sum_{k=1}^{n-1} {n-1 \choose k-1} k^{k-1} (n-k)^{n-k-1} \{\mu(k) + 1\}$$

for $n = 2, 3, \ldots$ ($\mu(1) = 0$ by definition). Let

$$M = M(x) = \sum_{n=2}^{\infty} \mu(n) n^{n-2} \frac{x^n}{(n-1)!}$$

and recall that the generating function

$$Y = Y(x) = \sum_{n=1}^{\infty} n^{n-2} \frac{x^n}{(n-1)!}$$

satisfies the relations

$$Y = xe^{Y}$$
 and $Y' = \frac{Y}{x(1-Y)}$

(Since $\mu(n) \le n - 1$, M(x) certainly converges if $|x| < e^{-1}$.) If we multiply equation (7.11) by $(n - 1)n^{n-2}x^n/(n - 1)!$ and sum over *n*, we obtain the relation

$$xM' - M = xM'Y + xY'Y$$

between M and Y. This may be rewritten as

$$(M/Y)' = Y'(1 - Y)^{-1},$$

from which it follows that

(7.12)
$$M = -Y \ln (1 - Y) = \sum_{j=1}^{\infty} \frac{1}{j} Y^{j+1}.$$

(The constant of integration must be zero since $\mu(1) = 0$.) If we use relation (4.2) to equate the coefficients of x^n in this equation, we obtain the required formula for $\mu(n)$.

Instead of determining the variance of λ directly, it is more convenient to determine $\tau(n)$, the expected value of $\lambda(\lambda - 1)$; the variance $\sigma^2(n)$ is then given by the formula $\sigma^2(n) = \tau(n) + \mu(n) - \mu^2(n)$.

THEOREM 7.15. If $n \ge 2$ and

$$\alpha_j = \sum_{i=1}^{j-1} \frac{1}{i}$$

for $j = 2, 3, ..., (\alpha_1 = 0)$, then

$$\tau(n) = 2 \sum_{j=1}^{n-1} \left(1 - \frac{1}{j} + \frac{\alpha_j}{j} \right) (j+1) \frac{(n-1)_j}{n^j}.$$

COROLLARY 7.15.1. As $n \to \infty$,

$$\sigma^2(n) = (2 - \frac{1}{2}\pi)n + O((n \log n)^{1/2})$$

It follows from equation (7.10) that

$$r(n) = \sum_{l=1}^{n-1} l(l-1)P(n,l)$$

= $\frac{1}{(n-1)n^{n-2}} \sum_{k=1}^{n-1} {n-1 \choose k-1} k^{k-1} (n-k)^{n-k-1} \{\tau(k) + 2\mu(k)\}$

for $n = 2, 3, ..., (\tau(1) = 0$ by definition). If we let

$$S = S(x) = \sum_{n=2}^{\infty} \tau(n) n^{n-2} \frac{x^n}{(n-1)!},$$

then it follows from the recurrence relation for $\tau(n)$ that

$$xS' - S = xS'Y + 2xM'Y.$$

This can be rewritten as

$$(S/Y)' = \frac{2}{1-Y}M' = 2Y'\{Y(1-Y)^{-2} - \ln(1-Y)\cdot(1-Y)^{-1}\};$$

consequently,

$$S = Y\{2Y(1 - Y)^{-1} + 2\ln(1 - Y) + \ln^2(1 - Y)\}$$
$$= 2\sum_{j=2}^{\infty} \left(1 - \frac{1}{j} + \frac{\alpha_j}{j}\right)Y^{j+1}.$$

If we equate the coefficients of x^n in this equation we obtain the required formula for $\tau(n)$.

The recurrence relation (7.10) can be used to express the generating functions of the numbers P(n, l) in terms of Y also, but the resulting expressions seem too complicated in general to be particularly useful; it can be shown, for example, that

$$P(n, 1) = (n - 1)^{n-3}/n^{n-2},$$

$$P(n, 2) = (5n + 1)(n - 2)(n - 1)^{n-5}/2n^{n-2},$$

and

$$P(n, 3) = (103n^{2} + 73n + 4)(n - 3)(n - 2)(n - 1)^{n-7}/(24n^{n-2}).$$

Theorem 3.3 states that if $1 \le t \le n$, then there are tn^{n-t-1} forests F_n of t trees with a total of n labelled nodes such that t given nodes, say the nodes 1, 2, ..., t, belong to different trees; we may consider these t nodes as the roots of the trees in F_n . Let $\mu(n, t)$ and $\tau(n, t)$ denote the expected value of λ and $\lambda(\lambda - 1)$ where $\lambda = \lambda(F_n)$ is the number of edges that must be removed from a random forest F_n of t rooted trees before isolating the t roots; at each stage the edge removed is chosen at random from the edges of the remaining subtrees containing the t roots.

If

$$M_{t} = \sum_{n=t+1}^{\infty} \mu(n, t) t n^{n-t-1} \frac{x^{n}}{(n-t)!}$$

and

$$S_t = \sum_{n=t+1}^{\infty} \tau(n, t) t n^{n-t-1} \frac{x^n}{(n-t)!}$$

then the argument used earlier in the case t = 1 can be extended to show that

$$M_t = -t Y^t \ln (1 - Y) = t \sum_{j=1}^{\infty} \frac{1}{j} Y^{j+t}$$

and

$$S_t = t Y^t \{ 2Y(1 - Y)^{-1} + 2\ln(1 - Y) + t\ln^2(1 - Y) \}$$
$$= 2t \sum_{j=2}^{\infty} \left(1 - \frac{1}{j} + \frac{t\alpha_j}{j} \right) Y^{j+t}$$

for t = 1, 2, ... If we equate the coefficients of x^n in these equations we obtain the following formulas for $\mu(n, t)$ and $\tau(n, t)$.

THEOREM 7.16. If $1 \le t \le n - 1$, then

$$\mu(n,t) = \sum_{j=1}^{n-t} \frac{j+t}{j} \cdot \frac{(n-t)_j}{n^j}$$

and

$$\tau(n,t) = 2\sum_{j=1}^{n-t} \left(1 - \frac{1}{j} + \frac{t\alpha_j}{j}\right)(j+t) \frac{(n-t)_j}{n^j}.$$

Notice that $M_t = t Y^{t-1}M_1$ and $S_t = t Y^{t-1}S_1$, so the numbers $\mu(n, t)$ and $\tau(n, t)$ can be expressed in terms of the numbers $\mu(m) = \mu(m, 1)$ and $\tau(m) = \tau(m, 1)$ for $2 \le m \le n - t + 1$.

Theorem 3.2 states that if $1 \le t \le n - 1$, then there are

$$\binom{n-2}{t-1}(n-1)^{n-t-1}$$

trees T_n in which the root x has degree t; let D(n, t) and U(n, t) denote the expected value of λ and $\lambda(\lambda - 1)$ for such trees. The argument used to establish equation (7.11) can be extended to show that

$$(7.13) \quad D(n,t) = \frac{1}{\binom{n-2}{t-1}(n-1)^{n-t}} \\ \times \left\{ \sum_{k=t+1}^{n-1} \binom{n-1}{k-1} \binom{k-2}{t-1} (k-1)^{k-t} (n-k)^{n-k-1} (D(k,t)+1) \right. \\ \left. + \sum_{k=t}^{n-1} \binom{n-1}{k-1} \binom{k-2}{t-2} (k-1)^{k-t} (n-k)^{n-k-1} (D(k,t-1)+1) \right\}$$

if $1 \le t \le n-1$ (otherwise D(n, t) = 0); the main difference is that now we must consider two possibilities when removing an edge e from a random tree T_n (in which d(x) = t) to obtain a subtree T_k containing the root x. If e is not incident with x then d(x) = t in T_k and e joins one of the k-1nodes of T_k other than x to one of the n - k nodes not in T_k ; if e is incident with x then d(x) = t - 1 in T_k and e joins x to one of the n - k nodes not in T_k . The two sums in the right hand side of equation (7.13) correspond to these two possibilities.

If

$$D_t = \sum_{n=t+1}^{\infty} D(n, t) {\binom{n-2}{t-1}} (n-1)^{n-t-1} \frac{x^{n-1}}{(n-1)!},$$

then it follows from equation (7.13) that

 $xD'_{t} = xD'_{t}Y + D_{t-1}Y + x(Y')' \cdot Y/t! + Y^{t-1} \cdot Y/(t-1)!,$

or equivalently, that

$$D'_{t} = \frac{1}{(t-1)!} Y^{t-1} \cdot Y'(1-Y)^{-1} + D_{t-1}Y'$$

~

for $t = 1, 2, \ldots$ The result

$$D_t = \frac{-1}{(t-1)!} Y^{t-1} \ln (1-Y) = \frac{1}{(t-1)!} \sum_{j=1}^{\infty} \frac{1}{j} Y^{j+t-1}$$

can now be established by induction if we use the fact that $D_t(0) = 0$ for all t and $D_0 = 0$. This implies the following formula.

THEOREM 7.17. If $0 \le t \le n - 1$, then

$$D(n + 1, t + 1) = \sum_{j=1}^{n-t} \frac{j+t}{j} \cdot \frac{(n-1-t)_{j-1}}{n^{j-1}}.$$

COROLLARY 7.17.1. If $1 \le t \le n - 1$, then

$$\mu(n, t) = \left(1 - \frac{t}{n}\right) D(n + 1, t + 1).$$

This corollary follows from Theorems 7.16 and 7.17; for fixed values of n, D(n + 1, t + 1) increases to n as t increases while $\mu(n, t)$ eventually decreases to 1.

If

$$U_t = \sum_{n=t+1}^{\infty} U(n, t) {\binom{n-2}{t-1}} (n-1)^{n-t-1} \frac{x^{n-1}}{(n-1)!},$$

then similar arguments can be used to show that

$$U_{t} = \frac{1}{(t-1)!} \times \{2Y^{t}(1-Y)^{-1} + 2Y^{t-1}\ln(1-Y) + (t-1)Y^{t-2}\ln^{2}(1-Y)\}$$
$$= \frac{2}{(t-1)!}\sum_{j=0}^{\infty} \left(1 - \frac{1}{j+1} + \frac{(t-1)\alpha_{j+2}}{j+2}\right)Y^{j+t}$$

for $t = 1, 2, \ldots$ This implies the following result.

THEOREM 7.18. If $1 \le t \le n - 1$, then

$$U(n,t) = 2 \sum_{j=0}^{n-1-t} \left(1 - \frac{1}{j+1} + \frac{(t-1)\alpha_{j+2}}{j+2}\right) \frac{(n-1-t)_j}{(n-1)^j}.$$

Notice that $(t-1)! \cdot D_t = Y^{t-1}D_1$ and $(t-1)! \cdot U_t = Y^{t-1}U_1 + (t-1)Y^{t-2}\ln^2(1-Y)$, so the numbers D(n, t) and U(n, t) can be expressed in terms of the numbers D(m, 1) and U(m, 1) for $2 \le m \le n - t + 1$.

96 Problems on Random Trees

THEOREM 7.19. If $0 \le t \le (n/\log n)^{1/2}$, then

 $D(n + 1, t + 1) = (\frac{1}{2}\pi n)^{1/2} + \frac{1}{2}t(\log n + 0(\log \log n)) + 0((\log n)^{1/2})$ as $n \to \infty$.

It follows from Theorem 7.17 that if $0 \le t \le n - 1$, then

$$D(n + 1, t + 1) = \sum_{k=0}^{n-t-1} \left(1 + \frac{t}{k+1}\right) C_k$$

where

$$C_k = \prod_{j=1}^k \left(1 - \frac{t+j}{n}\right).$$

Since $1 - x < e^{-x}$ for x > 0 it follows that

$$C_{\nu} \leq e^{-k^2/2n}$$

for all k; hence,

$$\sum_{k=0}^{n-t-1} C_k \leq 1 + n^{1/2} \int_0^\infty e^{-x^2/2} \, dx = 1 + (\frac{1}{2}\pi n)^{1/2}.$$

If $k \ge K = 2(n \log n)^{1/2}$, then $C_k \le 1/n^2$; hence,

$$\sum_{k=0}^{n-t-1} \frac{t}{k+1} C_k \le t \sum_{k=0}^{[K]-1} \frac{1}{k+1} + \frac{t}{n^2} \cdot \frac{n}{K} \le \frac{1}{2}t(\log n + \log \log n + 4)$$

for sufficiently large n. Therefore,

 $D(n + 1, t + 1) \le (\frac{1}{2}\pi n)^{1/2} + \frac{1}{2}t(\log n + \log \log n + 4) + 1$

if $0 \le t \le n - 1$ and n is sufficiently large.

It can also be shown that if $0 \le t \le (n/\log n)^{1/2}$ and n is sufficiently large, then

$$D(n + 1, t + 1) \ge (\frac{1}{2}\pi n)^{1/2} + \frac{1}{2}t(\log n - \log \log n - 5) - (\log n)^{1/2}.$$

The theorem now follows upon combining these two inequalities (see Meir and Moon (1970b) for the missing details). It follows from Corollary 7.17.1 that if $1 \le t \le (n/\log n)^{1/2}$ the conclusion of Theorem 7.19 remains valid if D(n + 1, t + 1) is replaced by $\mu(n, t)$; in particular, Corollary 7.14.1 holds. The average degree of the root in a random tree T_n is 2 - 2/nso perhaps it is not too surprising that $\mu(n) = \mu(n, 1)$ is asymptotically equal to D(n, 2) for large n. We now determine the asymptotic behaviour of the variance $\sigma^2(n)$ of λ for ordinary rooted trees T_n . It follows from Theorems 7.14 and 7.15 and the identity

$$\sum_{k=1}^n k(n)_k/n^k = n,$$

that

$$\tau(n) = 2(n-1) - 2\mu(n) + 2\sum_{k=1}^{n-1} \alpha_k \frac{k+1}{k} \cdot \frac{(n-1)_k}{n^k}.$$

If s_n denotes the last sum, then

$$s_n = \sum_{k=1}^{n-1} \{\log k + 0(1)\} \frac{k+1}{k} \frac{(n-1)_k}{n^k}$$

= $\{\frac{1}{2} \log n + 0(1)\} \mu(n) + \sum_{k=1}^{n-1} \log (kn^{-1/2}) \cdot \frac{k+1}{k} \cdot \frac{(n-1)_k}{n^k}.$

Now $(k + 1)/k \le 2$ and $(n - 1)_k/n^k < \exp(-k^2/2n)$; if the last sum is divided by $n^{1/2}$ it is bounded by an approximate Riemann sum for $\int_0^{\sqrt{n}} \log x \cdot e^{-x^2/2} dx$. Therefore,

$$\sigma^{2} = \tau(n) + \mu(n) - \mu^{2}(n)$$

= 2n + {log n + 0(1)} $\mu(n) - \mu^{2}(n) + 0(n^{1/2})$
= (2 - $\frac{1}{2}\pi$)n + 0((n log n)^{1/2})

as $n \to \infty$; this completes the proof of Corollary 7.15.1. More generally, it can be shown that if $1 \le t \le (n/\log n)^{1/2}$ then the variance of λ for forests F_n of t rooted trees or for trees T_n in which d(x) = t also equals $(2 - \frac{1}{2}\pi)n + o(n)$ as $n \to \infty$.

The entries in the following tables were computed by Mr. J. Hubert.

TABLE 5. Values of $\mu(n, t)$

n t	2	3	4	5	6	7	8	9	10
1	1	1.6667	2.1875	2.624	3.0046	3.3451	3.6551	3.9409	4.2072
2	_	1	1.75	2.36	2.8796	3.3357	3.7444	4.1163	4.4586
3			1	1.8	2.4722	3.0554	3.5728	4.0394	4.4656
4				1	1.8333	2.5510	3.1836	3.7508	4.2662
5					1	1.8571	2.6094	3.2812	3.8894
6						1	1.875	2.6543	3.358
7							1	1.8889	2.69
8								1	1.9
9									1

TABLE 6. Values of $D(n, t)$									
	2	3	4	5	6	7	8	9	10
-	1	1.5	1.8889	2.2185	2.5104	2.7747	3.0181	3.2450	3.4583
		2	2.5	2.9167	3.28	3.6056	3.9026	4.1772	4.4336
			3	3.5	3.9333	4.3194	4.6700	4.9925	5.2923
				4	4.5	4.9444	5.3469	5.7164	6.0591
					5	5.5	5.9524	6.3672	6.7514
						6	6.5	6.9583	7.3827
							7	7.5	7.9630
								8	8.5
									9

Let γ denote the number of edges that must be removed from a random tree T_n before separating two given nodes u and v, where at each stage the edge removed is chosen at random from the remaining subtree containing u and v. The preceding argument can be modified to show that the expected value of γ , given that the distance from u to v is d, is

$$1 + \sum_{t=1}^{n-1-d} \frac{1+d+t}{d+t} \frac{(n-1-d)_t}{n^t}$$

for $1 \le d \le n - 1$.

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99

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AUTHOR INDEX

van Aardene-Ehrenfest, T., 46, 51, 99 Anderson, S. S., 3, 99 Austin, T. L., 10, 17, 30, 31, 55, 70, 99

Bäbler, F., 6, 99
Baron, G., 65
Baum, L. E., 51, 99
Bedrosian, S. D., 15, 54, 57, 58, 61, 99, 103
Beineke, L. W., 16, 17, 21, 99
Bercovici, M., 57, 100
Berger, I., 51, 100
Blakely, G. R., 18, 68, 100
Bol, G., 22, 27, 28, 37, 100
Borchardt, C. W., 3, 11, 42, 100
Bott, R., 46, 100
Bromwich, J., 29, 82, 85, 100
Brooks, R. L., 41, 42, 100
Bryant, P. R., 39, 100

Cayley, A., 3, 4, 5, 11, 13, 42, 100 Char, J. P., 51, 100 Chen, W. K., 42, 47, 51, 100 Chistyakov, V. P., 74, 106 Chuard, J., 40, 100 Clarke, L. E., 14, 15, 17, 100

Dambit, Ja. Ja., 41, 65, 100 de Bruijn, N. G., 15, 46, 51, 99, 100 Dénes, J., 19, 22, 30, 68, 100, 101 Dixon, A. L., 42, 101 Duffin, R. J., 51, 101 Dziobek, O., 22, 23, 27, 28, 101

Eagon, J. A., 51, 99 Erdös, P., 82, 101

Fagen, R. E., 70, 99
Feussner, W., 51, 101
Fiedler, M., 10, 46, 47, 101
Ford, G. W., 33, 34, 37, 41, 80, 82, 101, 106, 107
Frame, J. S., 19

Gilbert, E. N., 23, 26, 101 Glicksman, S., 6, 8, 53, 101 Göbel, F., 15, 17, 53, 68, 101 Good, I. J., 37, 38, 55, 101 Groeneveld, J., 33, 82, 101,

Hadley, G. F., 46, 106 Hakimi, S. L., 6, 51, 101 Harary, F., 2, 3, 19, 20, 24, 99, 102 Harris, B., 66, 68, 78, 102 Helmer, R., 15, 102 Hubert, J., 77, 97 Husimi, K., 37, 102 Hutschenreuther, H., 41, 102

Kasai, T., 58, 60, 62, 102 Katz, L., 19, 66, 67, 102,

109

Kelmans, A. K., 42, 102 Kirchhoff, G., 1, 40, 42, 102 Klarner, D. A., 89 Klee, V., 10, 15, 103 Knuth, D. E., 3, 5, 8, 38, 46, 48, 51, 53, 103. König, D., 1, 79, 103 Kreweras, G., 37, 103 Kruskal, M. D., 69, 70, 103 Ku, Y. H., 42, 58, 103 Kusaka, H., 58, 60, 62, 102 Lantieri, J., 41, 103 Lempel, A., 6 Mallows, C. L., 32, 33, 103 Manvel. B., 3, 102 Matsui, K., 58, 102, Maxwell, J. C., 42, 103 Mayberry, J. P., 47, 100 Mayeda, W., 51, 103 Meir, A., 73, 74, 75, 76, 77, 90, 96, 103. Menon, V. V., 6, 14, 103 Moon, J. W., 6, 13, 16, 17, 21, 23, 31, 52, 64. 72, 73, 74, 75, 76, 77, 82, 85, 88, 90, 96, 99, 103, 104, Mowshowitz, A., 24, 102 Muir, T., 42, 104 Mukherjee, T., 51, 104 Mullin, R. C., 22, 104 Na. H. S., 63, 104 Nakagawa, N., 42, 43, 51, 58, 104 Neville, E. H., 5, 6, 104 Okada, S., 41, 104 Oláh, G., 55, 104 O'Neil, P. V., 55, 104 Onodera, R., 41, 104 Palásti, I., 82, 104 Palmer, E. M., 6, 7, 16, 20, 102, 104 Penny, W. E., 70, 99 Percival, W. S., 42, 104 Pippert, R. E., 16, 17, 99 Poincaré, H., 40, 104 Pólya, G., 22, 26, 30, 34, 104 Prins, G., 2, 102

Prüfer, H., 5, 6, 13, 15, 17, 21, 47, 53, 55. 104 Pullman, N. J., 85 Ramanujacharyulu, C., 6, 104 Raney, G. N., 10, 105 Rapoport, A., 63, 104 Read, R. C., 20, 102 Reed, M. B., 39, 106 Rénvi, A., 13, 17, 18, 20, 21, 28, 29, 41, 66, 67, 73, 74, 78, 79, 82, 101, 105 Riddell, R. J., 26, 105 Riordan, J., 3, 6, 7, 12, 18, 20, 24, 27, 30, 32, 33, 66, 69, 70, 78, 79, 99, 102, 103, 105 Robertson, M. M., 15, 105 Rohličkova, I., 9, 105 Rothe, R., 22 Rubin, H., 19, 68, 105 Sarker, P. K., 51, 104 Schoenfeld, L., 78, 102 Schützenberger, M. P., 7, 105 Scoins, H. I., 30, 105 Sedláček, J., 10, 46, 47, 53, 64, 65, 101, 106 Senior, J. K., 6, 106 Seshu, S., 39, 51, 103, 106 Sevast'vonov, B. A., 74, 106 Simmonard, M. A., 46, 106 Sitgreaves, R., 19, 68, 105 Slepian, P., 39, 55, 104, 106 Smith, C. A. B., 41, 42, 51, 100, 106 Sós, V. T., 21 Stanton, R. G., 22, 104 von Staudt, 1 Stone, A. H., 41, 42, 100 Suschkewitsch, A., 19, 106 Sylvester, J. J., 3, 42, 106 Szekeres, G., 78, 79, 105 Szwarc, W., 17, 106 Taki, I., 58, 60, 62, 102 Temperley, H. N. V., 33, 54, 80, 106 Thompson, J. J., 42 Trent, H. M., 41, 106 Tutte, W. T., 41, 42, 46, 51, 100, 106 Uhlenbeck, G. E., 26, 33, 34, 37, 41, 80, 82, 101, 105, 106, 107

Wang, K. T., 51, 107 Watson, G. N., 26, 107 Weinberg, L., 39, 42, 44, 53, 55, 63, 64, Weiss, I., 74, 107 Whittaker, E. T., 26, 107

107

Wintgen, G., 17, 106 Witzgall, C., 10, 15, 103 Yoneda, S., 58, 60, 62, 102 Zarankiewicz, C., 6, 107

SUBJECT INDEX

Arborescence, 6 Arc, 6, 7, 46, 48, 68 Automorphism group, 33

Block, 34

Characteristic polynomial, 42 Cluster integral, 80 Complement, 54, 58 Complexity of a graph, 80 Connected component, 1, 18, 25, 34, 40, 52, 54, 62, 70 Continuants, 58 Cycle, 1, 9, 18, 19, 36, 56, 58, 62, 67 Degree of a node, 1, 14, 70, 89, 94 Degree sequence, 6, 10, 13, 52, Determinant, 39, 40, 41, 47, 49 Diameter of a tree, 79 Distance between nodes, 1, 9, 76, 89, 98 Edge, 1, 41, 62, 83 Endnode, 1, 5, 6, 9, 20, 23, 32, 74, 86, 89 Eulerian circuit, 51 Foldant, 42, 51, 58 Forest, 10, 16, 17, 26, 27, 30, 42, 52, 81, 93 Functional digraph, 19, 66 Graph, arc-, 48 balanced, 47, 51

bipartite, 10, 55, 58, 62, 64 complete, 16, 37, 43, 53, 58, 60, 62, 63 connected, 1, 19, 23, 25, 34, 67, directed, 7, 18, 19, 22, 46, 48, 66 *k*-partite, 54, 56 labelled, 1 planar, 65 regular, 50, 65 rooted, 6, 26, 34 unlabelled, 1 Height of a tree, 78

Incidence matrix, 39 Incident edge or node, 1, 52 In-degree, 14, 48 Inversions, 32, 78 Isomorphic, 1, 34

Ladder, 64 Length of a path or cycle, 1, 19, 67 Loops, 7, 10, 11, 48,

Mapping function, 18, 19, 53, 66 Möbius ladder, 64

Node, 1, cut-, 34 root-, 6, 7, 8, 9, 20, 26, 47, 86, 90

Out-degree, 14, 47, 48

Subject Index 113

Path, 1, 56, 58, 68, 76 Permutation, 22, 32, 33, 70

Reduced incidence matrix, 40

Spanning subgraphs, 7 Spanning trees, 8, 41, 43, 47, 48, 52, 54, 80 Stirling numbers, 20, 37, 69, 74

Transposition, 22, 32 Tree, bicentred, 79 bipartite, 10, 21, 30, 37, 46, 55, 82 centred, 79 directed rooted, 6, 7, 8, 19, 47, 48, 68 k-, 16 oriented, 14 planted, 32 rooted, 17, 26, 32, 78, 86, 90 Tree function, 6, 8, 14 Tree polynomial, 42, 43, 51 Tree product, 41, 46

Unisignant, 42

Wheel, 64

112