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Combinatorial Theory

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3

Generating Functions and Recursions

3.1. RULES AND PROPERTIES

If $u_0, u_1, u_2, \ldots, u_n, \ldots$ is a sequence of numbers, we may associate with this sequence a *generating function* $g(x)$ by the rule

$$g(x) = u_0 + u_1 x + u_2 x^2 + \cdots + u_n x^n + \cdots. \tag{3.1.1}$$

If this series has a circle of convergence with a radius $R > 0$, then it may happen that the properties of the function $g(x)$ enable us to evaluate the coefficients u_n (or at least give estimates of their order of magnitude) or perhaps find other information of value. If $h(x)$ is the generating function of the sequence $v_0, v_1, v_2, \ldots, v_n, \ldots$, then

$$h(x) = v_0 + v_1 x + v_2 x^2 + \cdots + v_n x^n + \cdots. \tag{3.1.2}$$

If we add (3.1.1) multiplied by c, and (3.1.2) multiplied by d, we have

$$cg(x) + dh(x) = (cu_0 + dv_0) + (cu_1 + dv_1)x + \cdots + (cu_n + dv_n)x^n + \cdots, \tag{3.1.3}$$

and if we multiply, we have

$$g(x)h(x) = w_0 + w_1 x + w_2 x^2 + \cdots + w_n x^n + \cdots, \tag{3.1.4}$$

where for every $n = 1, 2, 3, \ldots$,

$$w_n = u_0 v_n + u_1 v_{n-1} + \cdots + u_{n-1} v_1 + u_n v_0. \tag{3.1.5}$$

Even if the series for $g(x)$ and $h(x)$ are not convergent, we may regard (3.1.3), (3.1.4), and (3.1.5) as defining formal operations on formal series. In these terms we easily verify that the addition, multiplication by scalars, and series multiplication satisfy the associative, commutative, and distributive laws. Furthermore, if $u_0 \neq 0$ and if we take $v_0 = u_0^{-1}$, we may use (3.1.5) to determine

$v_1, v_2, \ldots$ recursively to make $g(x)h(x) = 1$.

Instead of the generating function $g(x)$ associated with $u_0, u_1, \ldots, u_n, \ldots$, we may associate an *exponential generating function*, $G(x)$, by the rule

$$G(x) = u_0 + u_1 x + \frac{u_2 x^2}{2!} + \cdots + \frac{u_n x^n}{n!} + \cdots. \quad (3.1.6)$$

Similarly, let $H(x)$ be associated with $v_0, v_1, \ldots$ by

$$H(x) = v_0 + v_1 x + \frac{v_2 x^2}{2!} + \cdots + \frac{v_n x^n}{n!} + \cdots. \quad (3.1.7)$$

Then, for the product $G(x)H(x) = K(x)$,

$$G(x)H(x) = K(x) = w_0 + w_1 x + \frac{w_2 x^2}{2!} + \cdots + \frac{w_n x^n}{n!} + \cdots, \quad (3.1.8)$$

where

$$w_n = u_0 v_n + \binom{n}{1} u_1 v_{n-1} + \cdots + \binom{n}{r} u_r v_{n-r} + \cdots + \binom{n}{n} u_n v_0, \quad (3.1.9)$$

or symbolically,

$$w^n = (u + v)^n. \quad (3.1.10)$$

In the symbolic formula (3.1.10), it is to be understood that after expansion of $(u + v)^n$ by the binomial formula, all exponents are to be replaced by subscripts.

Suppose that a sequence $u_0, u_1, u_2, \ldots, u_n, \ldots$ satisfies the recurrence of rth order:

$$u_{n+r} = a_1 u_{n+r-1} + a_2 u_{n+r-2} + \cdots + a_r u_n, \qquad n = 0, 1, 2, \ldots, \quad (3.1.11)$$

where the a_i, $i = 1, \ldots, r$ are constants. Then, if $g(x)$ is the generating function for the sequence $\{u_n\}$, and if we take $k(x)$ as the polynomial

$$k(x) = 1 - a_1 x - a_2 x^2 - \cdots - a_r x^r, \quad (3.1.12)$$

we find that

$$g(x)k(x) = c_0 + c_1 x + c_2 x^2 + \cdots + c_{r-1} x^{r-1} = C(x), \quad (3.1.13)$$

where $C(x)$ is a polynomial of degree at most $r - 1$, since if c_{n+r} is the coefficient of x^{n+r}, $n \geqslant 0$, in the product $g(x)k(x)$, we find

$$c_{n+r} = u_{n+r} - a_1 u_{n+r-1} \cdots - a_r u_n = 0, \tag{3.1.14}$$

using the recursion (3.1.11). Thus, for a sequence $\{u_n\}$ satisfying the linear recurrence (3.1.11), the generating function $g(x)$ is a rational function

$$g(x) = \frac{C(x)}{k(x)}. \tag{3.1.15}$$

With the linear recurrence (3.1.11) we associate the *characteristic polynomial* $f(x)$ given by

$$f(x) = x^r - a_1 x^{r-1} - \cdots - a_r. \tag{3.1.16}$$

Without loss of generality we shall assume that $a_r \neq 0$, since if $a_r = 0$, the recurrence is not truly of order r but is of lower order. Let the factorization of $f(x)$ into linear factors be

$$f(x) = (x - \alpha_1)^{e_1}(x - \alpha_2)^{e_2} \cdots (x - \alpha_s)^{e_s}, \qquad e_1 + e_2 + \cdots + e_s = r, \tag{3.1.17}$$

where $\alpha_1, \ldots, \alpha_s$ are the (possibly) complex roots of $f(x)$. Comparing $f(x)$ of (3.1.16) and $k(x)$ of (3.1.12), we see that

$$k(x) = x^r f\left(\frac{1}{x}\right), \tag{3.1.18}$$

and corresponding to the factorization (3.1.17) of $f(x)$, we have the factorization of $k(x)$:

$$k(x) = (1 - \alpha_1 x)^{e_1} \cdots (1 - \alpha_s x)^{e_s}, \qquad e_1 + e_2 + \cdots + e_s = r. \tag{3.1.19}$$

We may express the rational function $g(x) = C(x)/k(x)$ in terms of partial fractions

$$g(x) = \frac{C(x)}{k(x)} = \sum_{i=1}^{s} \sum_{k=1}^{e_i} \frac{\beta_{ik}}{(1 - \alpha_i x)^k}, \tag{3.1.20}$$

where the β's are appropriate constants.

Thus, (3.1.20) expresses the generating function as a sum of functions of the form

$$\frac{\beta}{(1 - \alpha x)^k} = \beta(1 - \alpha x)^{-k}. \tag{3.1.21}$$

We may easily expand (3.1.21) by the binomial formula to find

$$\beta(1-\alpha x)^{-k} = \beta\left(1 + (-k)(-\alpha x) + \cdots + \frac{(-k)\cdots(-k-n+1)(-\alpha x)^n}{n!} + \cdots\right). \tag{3.1.22}$$

In this, the coefficient of x^n is

$$\frac{\beta(n+k-1)\cdots(k)}{n!}\alpha^n = \beta\binom{n+k-1}{n}\alpha^n = \beta\binom{n+k-1}{k-1}\alpha^n. \tag{3.1.23}$$

We note that

$$\sum_{k=1}^{e_i} \beta_{ik}\binom{n+k-1}{k-1}\alpha_i^n = P_i(n)\alpha_i^n, \tag{3.1.24}$$

where $P_i(n)$ is a polynomial of degree at most $e_i - 1$ in n, and that any polynomial $P_i(n)$ can be obtained by using an appropriate choice of constants β_{ik}. Substituting back in (3.1.20), we have

$$\begin{aligned} g(x) &= \sum_{n=0}^{\infty} u_n x^n \\ &= \sum_{n=0}^{\infty}\sum_{i=1}^{s} P_i(n)\alpha_i^n x^n, \end{aligned} \tag{3.1.25}$$

and comparing coefficients of x^n, we have

$$u_n = \sum_{i=1}^{s} P_i(n)\alpha_i^n, \tag{3.1.26}$$

where $P_i(n)$ is degree at most $e_i - 1$.

We shall state this result as a theorem.

Theorem 3.1.1. *Suppose a sequence $u_0, u_1, u_2, \ldots, u_n, \ldots$ satisfies the linear recurrence with constant coefficients*

$$u_{n+r} = a_1 u_{n+r-1} + \cdots + a_r u_n, \qquad n \geqslant 0.$$

Let us call $f(x) = x^r - a_1 x^{r-1} - \cdots - a_r$ the characteristic polynomial of this *recurrence and let*

$$f(x) = (x - \alpha_1)^{e_1} \cdots (x - \alpha_s)^{e_s}, \qquad e_1 + e_2 + \cdots + e_s = r$$

be the factorization of $f(x)$ *as a product of linear factors. Then*

$$u_n = \sum_{i=1}^{s} P_i(n)\alpha_i^n$$

for all n, where $P_i(n)$ *is a polynomial of degree at most* $e_i - 1$ *in n. The coefficients of the polynomials* $P_i(n)$ *are determined by the initial values* $u_0, u_1, \ldots, u_{r-1}$ *of the sequence* $\{u_n\}$.

3.2. COMBINATORIAL PROBLEMS

Let us consider a combinatorial problem whose solution depends on a linear recurrence. Let u_t, $t \geqslant 2$, be the number of ways of finding a permutation $a_1a_2, \ldots, a_t$ of $1, 2, \ldots, t$ such that for each i, a_i is in the ith column of the array:

$$\begin{array}{ccccccc} & 1 & 2 & \cdots & t-3 & t-2 & t-1 \\ 1 & 2 & 3 & \cdots & t-2 & t-1 & t \\ 2 & 3 & 4 & \cdots & t-1 & t & \end{array} \tag{3.2.1}$$

Here we find directly that $u_2 = 2$, $u_3 = 3$, $u_4 = 5$. The number t must be used in either the tth or $(t-1)$th column. Thus, our two choices are

$$\begin{array}{cccccc} & 1 & 2 & \cdots & t-3 & t-2 & \bigcirc\!\!\!\!\!\;t \\ 1 & 2 & 3 & \cdots & t-2 & t-1 & \\ 2 & 3 & 4 & \cdots & t-1 & & \end{array} \tag{3.2.2}$$

or

$$\begin{array}{ccccccc} & 1 & 2 & \cdots & t-3 & \bigcirc\!\!\!\!\!\;t & \boxed{t-1} \\ 1 & 2 & 3 & \cdots & t-2 & & \\ 2 & 3 & 4 & \cdots & & & \end{array} \tag{3.2.3}$$

In both cases chosen numbers have been circled. In (3.2.2) we have omitted the t from the $(t-1)$th column, since it cannot be used there. In (3.2.3), having chosen t from the $(t-1)$th column, we must choose $t-1$ from the tth column and then omit $t-1$ from the $(t-2)$th column. The number of choices in (3.2.2) for $1, 2, \ldots, t-1$ is u_{t-1}, and the number of choices in (3.2.3) is u_{t-2}. Hence, as these combine to give all choices in (3.2.1), we have

$$u_t = u_{t-1} + u_{t-2}, \tag{3.2.4}$$

a linear recurrence of second order for u_t. Although the combinatorial problem is not meaningful for $t = 0$ or 1, the values $u_0 = 1$, $u_1 = 1$ are consistent with the recurrence (3.2.4) and the succession of values $u_0 = 1$, $u_1 = 1$, $u_2 = 2$, $u_3 = 3$, $u_4 = 5, \ldots$. The characteristic polynomial of (3.2.4) is

$$f(x) = x^2 - x - 1 = (x - \alpha_1)(x - \alpha_2), \tag{3.2.5}$$

where

$$\alpha_1 = \frac{1 + \sqrt{5}}{2}, \qquad \alpha_2 = \frac{1 - \sqrt{5}}{2}. \tag{3.2.6}$$

We easily find from Theorem 3.1.1 and our initial values that

$$u_n = \frac{1}{\sqrt{5}} \cdot (\alpha_1^{n+1} - \alpha_2^{n+1}). \tag{3.2.7}$$

Another, more natural, combinatorial problem can be reduced to the evaluation of u_t just made. What is the number z_n, $n \geqslant 3$, of permutations $a_1 a_2 \cdots a_n$ of $1, 2, \ldots, n$ such that a_i is in the ith column of the following array?

$$\begin{array}{ccccccc} 1 & 2 & 3 & \cdots & n-3 & n-2 & n-1 & n \\ 2 & 3 & 4 & \cdots & n-2 & n-1 & n & 1 \\ 3 & 4 & 5 & \cdots & n-1 & n & 1 & 2 \end{array} \tag{3.2.8}$$

The complete set of choices can be subdivided according to the choice of column in which n is selected, and if this is not the $(n-1)$th column, the choice of $n-1$ or 1 is in the $(n-1)$th column. These choices may be indicated by the circled values shown in the last three columns as follows:

$$\text{(a)}\ \begin{array}{ccc} n-2 & \textcircled{$n-1$} & \textcircled{n} \\ n-1 & n & 1 \\ n & 1 & 2 \end{array} \qquad \text{(b)}\ \begin{array}{ccc} n-2 & n-1 & \textcircled{n} \\ n-1 & n & 1 \\ n & \textcircled{1} & 2 \end{array}$$

$$\text{(c)}\ \begin{array}{ccc} n-2 & n-1 & n \\ n-1 & \textcircled{n} & 1 \\ n & 1 & 2 \end{array} \qquad \text{(d)}\ \begin{array}{ccc} n-2 & n-1 & n \\ n-1 & n & 1 \\ \textcircled{n} & \textcircled{1} & 2 \end{array} \qquad \text{(e)}\ \begin{array}{ccc} n-2 & \textcircled{$n-1$} & n \\ n-1 & n & 1 \\ \textcircled{n} & 1 & 2 \end{array} \tag{3.2.9}$$

In case (a) there is exactly one choice, namely, the top row of (3.2.8), for only a single 1 remains to be chosen, and this is in the first column. Having chosen this 1, only the 2 in the second column remains, and similarly the choices of $3, 4, \ldots, n-2$ in the first row are forced. In case (b) we are to choose from

$$\begin{matrix} & 2 & 3 & \cdots & n-3 & n-2 \\ 2 & 3 & 4 & \cdots & n-2 & n-1 \\ 3 & 4 & 5 & \cdots & n-1 & \end{matrix} \tag{3.2.10}$$

and this number is u_{n-2}. In (c) the choices are from the array for u_{n-1}. In (d) there is exactly one choice, namely, the third row, since only one $n-1$ remains to be chosen and that is in the $(n-3)$th column; similarly, the $n-2, n-3, \ldots, 2$ in the third row must be chosen. In (e) the choices are from the array for u_{n-2}. Hence, the total number of choices for (3.2.8), z_n, is given by

$$\begin{aligned} z_n &= 1 + u_{n-2} + u_{n-1} + 1 + u_{n-2} \\ &= u_n + u_{n-2} + 2 \\ &= \alpha_1^n + \alpha_2^n + 2, \end{aligned} \tag{3.2.11}$$

where

$$\alpha_1 = \frac{1+\sqrt{5}}{2}, \qquad \alpha_2 = \frac{1-\sqrt{5}}{2}$$

as before.

The number u_n of derangements of $1, 2, \ldots, n$ evaluated in (2.1.6) may also be found recursively. Consider a derangement

$$\begin{pmatrix} 1 & 2 & \cdots & n \\ a_1 & a_2 & \cdots & a_n \end{pmatrix}. \tag{3.2.12}$$

If $a_1 = j$, we consider the partial permutation

$$\begin{pmatrix} 2 & \cdots & j & \cdots & n \\ a_2 & \cdots & a_j & \cdots & a_n \end{pmatrix}. \tag{3.2.13}$$

Two cases are to be considered here. First are cases with $a_j \neq 1$, and second those with $a_j = 1$. These cases are collectively exhaustive and mutually exclusive. In the first case we have

$$\begin{pmatrix} 2 & \cdots & i & \cdots & j & \cdots & n \\ a_2 & \cdots & 1 & \cdots & a_j & \cdots & a_n \end{pmatrix}, \qquad i \neq j, \tag{3.2.14}$$

which may be associated with the derangement of $2, \ldots, n$:

$$\begin{pmatrix} 2 & \cdots & i & \cdots & j & \cdots & n \\ a_2 & \cdots & j & \cdots & a_j & \cdots & a_n \end{pmatrix}. \tag{3.2.15}$$

Conversely, every derangement of $2, \ldots, n$ such as (3.2.15) leads to $(n-1)$ derangements of $1, 2, \ldots, n$ of this first kind by taking j as $2, \ldots, n$ in turn. In the second case, with $a_j = 1$, the partial permutation of (3.2.13) takes the form

$$\begin{pmatrix} 2 & \cdots & j & \cdots & n \\ a_2 & \cdots & 1 & \cdots & a_n \end{pmatrix}. \tag{3.2.16}$$

If we delete the $\binom{j}{1}$, this is a derangement of $2, \ldots, j-1, j+1, \ldots, n$; conversely, for each $j = 2, \ldots, n$, such derangements of $(n-2)$ numbers lead to derangements of $1, \ldots, n$ of the second type. These two cases combine to give us the recursion

$$u_n = (n-1)u_{n-1} + (n-1)u_{n-2}. \tag{3.2.17}$$

We may easily verify that this recursion yields thc same numbers as (2.1.6).

A sequence $x_1 x_2 \cdots x_n$ may be combined in this order by a binary non-associative product in a number of ways. What is this number u_n? For $n = 3, 4$ we have the possibilities

$$\begin{aligned} &x_1(x_2x_3), && (x_1x_2)x_3; \\ &x_1(x_2(x_3x_4)), && x_1((x_2x_3)x_4); \\ &(x_1x_2); (x_3x_4) && \\ &(x_1(x_2x_3))x_4, && ((x_1x_2)x_3)x_4. \end{aligned} \tag{3.2.18}$$

Thus, $u_3 = 2$, $u_4 = 5$. We also have $u_2 = 1$ and will take $u_1 = 1$ as a convention. The last product will be some composite of the first r letters multiplied by some composite of the last $(n-r)$, of the form $(a_1 \cdots a_r)(a_{r+1} \cdots a_n)$. The first r can be combined in u_r ways (here the convention $u_1 = 1$ fits) and the last $(n-r)$ in u_{n-r} ways. Thus

$$u_n = u_1 u_{n-1} + u_2 u_{n-2} + \cdots + u_{n-1} u_1, \qquad n \geqslant 2. \tag{3.2.19}$$

Let us write the generating function $f(x)$ as

$$f(x) = u_1 x + u_2 x^2 + \cdots + u_n x^n + \cdots, \tag{3.2.20}$$

postponing the consideration of its convergence. The recursion (3.2.19) is equivalent formally to the relation

$$(f(x))^2 = -x + f(x) \tag{3.2.21}$$

We note that $u_1 = 1$ and that the recursion (3.2.19) holds only for $n \geq 2$ and must account for this by the $-x$ on the right-hand side of (3.2.21). Solving (3.2.21) for $f(x)$ as a quadratic equation, we have

$$f(x) = \frac{1 - \sqrt{1 - 4x}}{2}. \tag{3.2.22}$$

Here we take the minus sign, since the series for $f(x)$ has no constant term. Expanding (3.2.22) as a power series, we find the coefficient of x^n to be v_n, where

$$v_n = \frac{(\frac{1}{2})(-\frac{1}{2})\cdots((3 - 2n)/2)(-4)^n(-\frac{1}{2})}{n!}. \tag{3.2.23}$$

This simplifies to

$$v_n = \frac{(2n - 2)!}{n!(n - 1)!}. \tag{3.2.24}$$

We may now observe that the series for $f(x)$ as given by (3.2.22) must converge for $|x| < \frac{1}{4}$, and for these values the equation (3.2.21)—and hence the recursion (3.2.19)—with v_n in place of u_n must hold. But as $u_1 = v_1 = 1$, we have $u_n = v_n$ for all $n \geq 1$, and so our solution is

$$u_n = \frac{(2n - 2)!}{n!(n - 1)!} \tag{3.2.25}$$

for all $n \geq 2$. We observe that an attempt to prove the convergence of (3.2.20) on the basis of (3.2.19) alone is exceedingly difficult.

PROBLEMS

1. The Fibonacci numbers are the sequence of numbers $u_0, u_1, \ldots, u_n, \ldots$ with $u_0 = 0$, $u_1 = 1$, and $u_{n+2} = u_{n+1} + u_n$. Show that every positive integer N has a unique representation

$$N = \sum_{i=1}^{\infty} a_i u_i$$

with $a_i = 0$ or 1 and $a_i a_{i+1} = 0$, $i \geq 1$.

2. Numbers $s(n, r)$ and $S(n, r)$, called the Stirling numbers of the first and second kind, respectively, are defined by the rules

$$(x)_n = x(x-1)\cdots(x-n+1) = \sum_{r=0}^{n} s(n, r)x^r, \qquad n > 0$$

and

$$x^n = \sum_{r=0}^{n} S(n, r)(x)_r, \qquad n > 0.$$

Here we take $x^0 = (x)_0 = 1$. Show that

$$\sum_r S(n, r)s(r, m) = \delta_{nm},$$

the Kronecker delta, where $\delta_{nn} = 1$, $\delta_{nm} = 0$ if $n \neq m$. From this, show that each of the two relations

(a) $$a_n = \sum_r s(n, r)b_r, \qquad n = 1, 2, \ldots,$$

(b) $$b_n = \sum_r S(n, r)a_r, \qquad n = 1, 2, \ldots,$$

implies the other.

3. Use the relation $(x)_{m+1} = (x - m)(x)_m$ to derive the recursions for the Stirling numbers of the first and second kind:

$$s(n + 1, r) = s(n, r - 1) - ns(n, r),$$

$$S(n + 1, r) = S(n, r - 1) + rS(n, r).$$

4. Let $P_n = \sum_{r=0}^{n} (n)_r$, this being the total number of permutations of n distinct objects, without repetitions.

   (a) Show that P_n satisfies the recurrence $P_n = nP_{n-1} + 1$, $n \geqslant 1$, $P_0 = 1$.

   (b) Show that $P_n = n! \sum_{r=0}^{n} 1/r!$ and conclude that for $n \geqslant 2$, P_n is the nearest integer to $n!e$.

   (c) Show that $\sum_{n=0}^{\infty} P_n x^n/n! = e^x/(1 - x)$.

5. A Dirichlet generating function $A(s)$ for a sequence of numbers $a_1, a_2, \ldots$ is a formal series

$$A(s) = \sum_{n=1}^{\infty} \frac{a_n}{n^s}.$$

If

$$B(s) = \sum_{n=1}^{\infty} \frac{b_n}{n^s},$$

we define

$$A(s) + B(s) = C(s) = \sum_{n=1}^{\infty} \frac{c_n}{n^s},$$

where $c_n = a_n + b_n$ and

$$A(s)B(s) = V(s) = \sum_{n=1}^{\infty} \frac{v_n}{n^s},$$

where

$$v_n = \sum_{d|n} \frac{a_d b_{n/d}}{d}.$$

(a) Prove that this product rule is commutative and associative.
(b) Show that if $i_1 = 1, 0 = i_2 = i_3 = \cdots$, the series $I(s)$ is a unit for this multiplication.
(c) Show that if $a_1 \neq 0$, the series $A(s)$ has an inverse $B(s)$ satisfying

$$A(s)B(s) = I(s).$$

6. Define the zeta function as

$$\zeta(s) = \sum_{n=1}^{\infty} \frac{1}{n^s}.$$

Show that the inverse of $\zeta(s)$ is the series

$$\zeta(s)^{-1} = \sum_{n=1}^{\infty} \frac{\mu(n)}{n^s},$$

where the function $\mu(n)$ is the Möbius function defined in (2.1.10). If $a_n = g(n)$, $b_n = f(n)$ for all n, and $B(s) = A(s)\zeta(s)$, then $A(s) = B(s)\zeta(s)^{-1}$. Show that this corresponds to the Möbius inversion formula of Theorem 2.1.1.