Chapter 3

Evaluating Sums

The concern of this chapter is a collection of methods for the evaluation of a finite sum whose summands are given as a sequence, either in a functional form $f(k)$, or in a subscripted form x_k. Analogous to the sense in which a real function may have for its *integral* over an interval an anti-derivative function evaluated at the bounds of the interval, the value of such a finite sum may be given by some other function of the lower and upper limits of the index k.

REVIEW FROM §1.4:

- Let $\langle x_n \rangle$ be a sequence. Then the expression

$$\sum_{j=0}^{n} x_j = x_0 + x_1 + \cdots + x_n \tag{3.0.1}$$

(and also its value) are called the n^{th} ***partial sum***.

NOTATION: Sometimes S_n denotes the n^{th} partial sum.

3.1 NORMALIZING SUMMATIONS

DEF: A ***consecutive summation*** is an expression

$$\sum_{k=a}^{b} x_k$$

where a and b be integers or integer-valued variables, and where $\langle x_n \rangle$ is a sequence with its values in an algebraic structure (e.g., the integers, reals, or complex numbers) with an associative and commutative addition. Its value, the ***sum***, is defined recursively.

$$\sum_{k=a}^{b} x_k = \begin{cases} 0 & \text{if } b < a \\ x_a & \text{if } b = a \\ \left(\sum_{k=a}^{b-1} x_k \right) + x_b & \text{if } b > a \end{cases}$$

The parameters of the expression have names:

- k is called the ***index variable***;
- a is called the ***lower limit*** of the index;
- b is called the ***upper limit*** of the index;
- x_k is called the ***summand.***

If the lower limit a and the upper limit b are both given as fixed integers, then the sum has a ***definite value*** within the domain of its summands. For instance, if the summands are integers, then the sum is an integer.

Example 3.1.1: $$\sum_{k=0}^{2} k^2 \;=\; 0^2 + 1^2 + 2^2 \;=\; 5. \qquad (3.1.2)$$

Quite commonly, a summation has a lower index limit fixed at 0 and a symbolic upper limit of n, in which case summation may be regarded as an operator on a sequence

$$\langle x_n \mid n \;=\; 0,\, 1,\, \ldots \rangle$$

whose application produces a sequence of partial sums

$$\left\langle \sum_{j=0}^{n} x_j \;\middle|\; n \;=\; 0,\, 1,\, \ldots \right\rangle$$

akin to the way that integration operates on a function to produce a new function. This chapter develops methods for ***evaluating the summation***, which, in this context, often means producing a closed formula for the elements of the sequence of partial sums.

Example 3.1.1, cont.: With the variable n as the upper limit, the value of the sum of the form (3.1.2) is

$$\sum_{k=0}^{n} k^2 \;=\; \frac{2n^3 + 3n^2 + n}{6}$$

This formula could be confirmed immediately by mathematical induction, or by any of the methods of summation to be introduced in subsequent sections of this chapter.

Sums over Sets

In a more general context, the *indexing set* of a given summation may be any finite set T. Given any function f with values in $\mathbb{Z}$, $\mathbb{Q}$, $\mathbb{R}$, or $\mathbb{C}$, the sum

$$\sum_{y \in T} f(t)$$

is well-defined. In a sum over an unordered indexing set, the order in which the index variable t takes its values is not specified or implied, and the value would be the same for any order of summation.

Example 3.1.2: The sum of the weights of the edges in the graph G of Fig 3.1.1 is represented by the expression

$$\sum_{e \in E_G} w(e)$$

whose value is

$$6 + 7 + 3 + 2 + 3 + 6 + 5 + 5 + 6 + 4 + 10 + 5 \;=\; 62$$

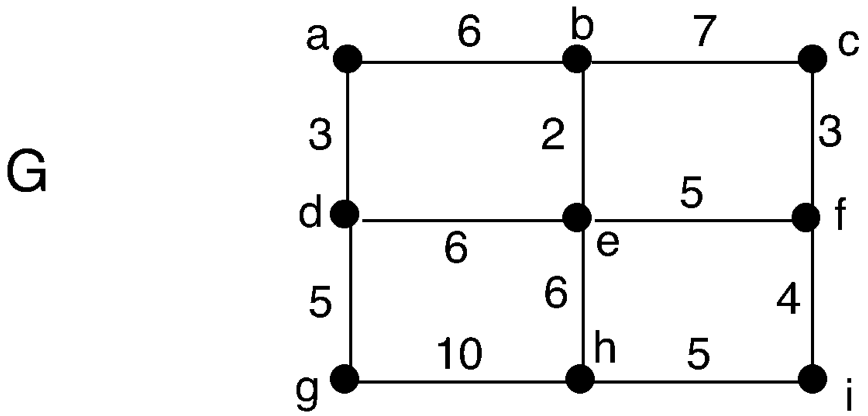

Fig 3.1.1 **An edge-weighted graph.**

In principle, the edges of the graph G could be indexed by integers $0, 1, \ldots, 11$, which would permit the sum of their weights to be represented by a consecutive summation. There seems to be little gained from doing so in this example. Our focus here is to do something more efficient, when possible, than successively incrementing a running total by additional summands. Such tedium is unavoidable when the summands have no discernable pattern, especially if the summands are random numbers. However, in many other cases, when the index set is a subset of the integers, a transformation may simplify the evaluation.

DEF: Indexing the summands over consecutive integers is called ***normalizing a summation.***

Example 3.1.3: The sum

$$\sum_{\substack{1 \le k < 20 \\ k \text{ odd}}} k$$

can be normalized to

$$\sum_{k=0}^{9} (2k+1)$$

which is readily transformed further into

$$\sum_{k=0}^{9} (2k+1) \;=\; \sum_{k=0}^{9} 2k \;+\; \sum_{k=0}^{9} 1$$

$$= 2\sum_{k=0}^{9} k + 10$$

$$= 2 \cdot \frac{10^{\underline{2}}}{2} + 10 \qquad \text{(by Corollary 1.5.2)}$$

$$= 10^{\underline{2}} + 10$$

$$= 100$$

Many of the methods to be introduced in this chapter are designed to work on normalized summations. Other sums are transformed into consecutive sums to permit the application of such methods.

Iverson Truth Function

When the index variable of a summation has irregular gaps in its range, it may still be possible to normalize, by inserting into the summand an artificial multiplier that effectively cancels the summand across the gaps.

Example 3.1.4: For instance, the index variable p of the sum

$$\sum_{\substack{p \le n \\ p \text{ prime}}} \sqrt{p} \qquad (3.1.3)$$

has gaps between consecutive primes.

DEF: The ***Iverson truth function*** is defined by the rule

$$(\text{predicate}) = \begin{cases} 1 & \text{if the predicate is true} \\ 0 & \text{if the predicate is false} \end{cases}$$

Example 3.1.4, cont.: Using the Iverson truth function facilitates the reformulation of (3.1.3) as a consecutive summation.

$$\sum_{\substack{p \leq n \\ p \text{ prime}}} \sqrt{p} \quad = \quad \sum_{p=1}^{n} \left[(p \text{ prime}) \cdot \sqrt{p} \, \right]$$

CONVENTION: The value of the product

$$(P(k)) \cdot a_k$$

is 0 whenever the value of the Iverson expression $(P(k))$ is 0, even when a_k is undefined.

Example 3.1.5: The value of the sum

$$\sum_{p=0}^{n} \frac{1}{p} \cdot (p \text{ prime})$$

is well-defined, since the "strong zero" of the Iverson expression (p prime) cancels the effect of the undefined quotient $\frac{1}{p}$ when $p = 0$.

Algebraic Regrouping

Part of the art of simplifying and evaluating sums is to manipulate them so that recognizable forms emerge. The familiar algebraic properties of the number system include several principles for regrouping. These principles are applied independently and also in conjunction with the other summation methods of this chapter.

Proposition 3.1.1 [Distributive Law]. *A common factor can be distributed over all the summands.*

$$\sum_{k \in K} c a_k \;=\; c \sum_{k \in K} a_k$$

Proposition 3.1.2 [Addition Law]. *Two sums over the same index set can be combined into a single sum by adding each pair of summands with the same index.*

$$\sum_{k \in K} (a_k + b_k) \;=\; \sum_{k \in K} a_k + \sum_{k \in K} b_k$$

Proposition 3.1.3 [Permutation Law]. *The value of a sum is unchanged by permuting the order of the summands.*

$$\sum_{k \in K} a_k \;=\; \sum_{k \in K} a_{\pi(k)}$$

As a first illustration, we apply these algebraic regroupings to an *arithmetic progression*. From our present perspective, that means a sequence $\langle a_n \rangle$ given by a recurrence of the form

$$\begin{aligned} a_0 &= c \\ a_n &= a_{n-1} + b \qquad \text{for } n > 0 \end{aligned}$$

For instance, the consecutive odd numbers $3, 5, 7, 9, \ldots$ are an arithmetic progression, with initial value $c = 3$ and increment $b = 2$.

Example 3.1.6: Simplifying the sum of a finite arithmetic progression

$$S_n = \sum_{k=0}^{n} (c + bk) \qquad (3.1.4)$$

can begin with application of the Permutation Law.

$$S_n = \sum_{k=0}^{n} (c + b(n-k)) \qquad (3.1.5)$$

Adding equations (3.1.4) and (3.1.5) leads into the following analysis.

$$\begin{aligned}
2S_n &= \sum_{k=0}^{n} (c + bk) + \sum_{k=0}^{n} (c + b(n-k)) \\
&= \sum_{k=0}^{n} [(c + bk) + (c + b(n-k))] && \text{(Addition Law)} \\
&= \sum_{k=0}^{n} (2c + bn) \\
&= (2c + bn) \sum_{k=0}^{n} 1 && \text{(Distributive Law)} \\
&= (2c + bn)(n+1) \\
\Rightarrow S_n &= \left(c + \frac{bn}{2}\right) \cdot (n+1) && (3.1.6)
\end{aligned}$$

Example 3.1.7: This is a special case of formula (3.1.6).

$$\begin{aligned}\sum_{k=0}^{n} k &= \left(0 + \frac{1 \cdot n}{2}\right) \cdot (n+1) \\ &= \left(\frac{n}{2}\right) \cdot (n+1) \\ &= \binom{n+1}{2}\end{aligned}$$

For instance,

$$0+1+2+3+4+5 \;=\; 15 \;=\; \binom{6}{2}$$

Harmonic Numbers

REVIEW FROM §1.2:

> The sequence of ***harmonic numbers*** $\langle H_n \rangle$ is defined by the rule
>
> $$\begin{aligned} H_n &= \sum_{k=1}^{n} \frac{1}{k} \\ &= \frac{1}{1} + \frac{1}{2} + \cdots + \frac{1}{n} \qquad \text{for } n \geq 0 \end{aligned}$$

The harmonic numbers are the discrete analogue of the natural logarithm

$$\ln(n) \;=\; \int_1^n \frac{1}{x}\,dx$$

Figure 3.1.2 illustrates that the harmonic number and the natural logarithm are reasonably good approximations of each other. Familiarity with upper and lower Riemann sums may add some interest here, but such familiarity is not necessary for understanding of the correctness of the approximation.

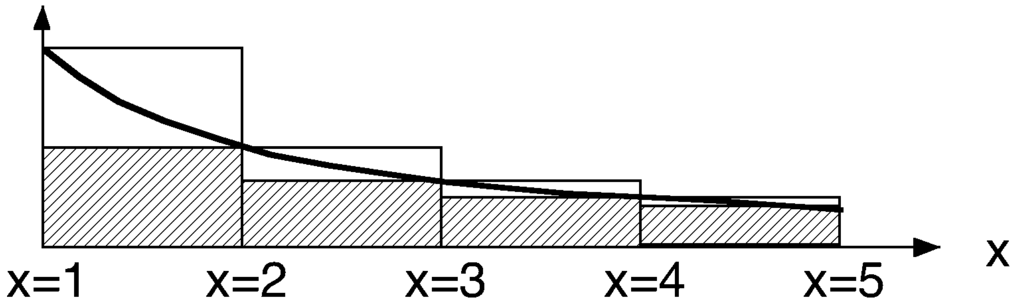

Fig 3.1.2 Upper and lower Riemann approximations of $\frac{1}{x}$.

Since the area under the curve $1/x$ over the interval $[1, 5]$ is $\ln(5)$, one observes that $\ln 5$ is less than the sum of the areas of the upper rectangles, i.e.,

$$\ln 5 \ < \ \frac{1}{1} + \frac{1}{2} + \frac{1}{3} + \frac{1}{4} \ = \ H_4 \qquad \text{upper sum}$$

and that $\ln 5$ is greater than the sum of the areas of the lower rectangles, i.e.,

$$H_5 - 1 \ = \ \frac{1}{2} + \frac{1}{3} + \frac{1}{4} + \frac{1}{5} \ < \ \ln 5 \qquad \text{lower sum}$$

This observation generalizes to the following:

Proposition 3.1.4. *For any positive integer n*

$$\text{(a)}\quad \ln(n+1) \;<\; H_n \;<\; \ln(n) + 1$$
$$\text{(b)}\quad H_n - 1 \;<\; \ln(n) \;<\; H_{n-1}$$

Proof: Summing the areas of the upper rectangles (i.e., taking upper Riemann sums) yields

$$\ln(n+1) \;<\; \frac{1}{1} + \cdots + \frac{1}{n} \;=\; H_n \qquad (3.1.7)$$
$$\ln(n) \;<\; \frac{1}{1} + \cdots + \frac{1}{n-1} \;=\; H_{n-1} \qquad (3.1.8)$$

and summing the areas of the lower rectangles (i.e., taking lower Riemann sums) yields

$$H_n - 1 \;=\; \frac{1}{2} + \cdots + \frac{1}{n-1} \;<\; \ln n \qquad (3.1.9)$$

Together, (3.1.7) and (3.1.9) imply part (a). Similarly, (3.1.9) and (3.1.8) imply part (b). ◊

GKP Notations

DEF: Let n and d be integers. If there is an integer q such that $n = dq$, then we say that d ***divides*** n. Notation: $d \backslash n$.

DEF: Let m and n be integers whose greatest common divisor is 1. Then we say that m and n are ***relatively prime***. Notation $m \perp n$.

3.2 PERTURBATION

The initial step of a ***perturbation*** is to equate two expressions for S_{n+1}, the $n+1^{\text{st}}$ partial sum of the sequence $\langle x_n \rangle$.

$$S_n + x_{n+1} = x_0 + \sum_{k=1}^{n+1} x_k$$

The sums on both sides of the equal sign are clearly equal. Perturbation is a practical method, and additional tricks are used as needed. What makes it interesting is not the theory behind it, but the fact that it works so effectively so often.

Example 3.2.1: A very simple first example of applying perturbation is to evaluate the summation

$$S_n = \sum_{k=0}^{n} 2^k \qquad (3.2.1)$$

Of course, the solution to the summation (3.2.1) is easily obtainable by other methods, but the details serve as a good illustration of the technique of perturbation.

$$\begin{aligned}
S_n + 2^{n+1} &= 2^0 + \sum_{k=1}^{n+1} 2^k \;=\; 1 + \sum_{k=1}^{n+1} 2^k && \text{(set up)} \\
&= 1 + \sum_{k=0}^{n} 2^{k+1} && \text{(change of limits)} \\
&= 1 + 2\sum_{k=0}^{n} 2^k \\
&= 1 + 2S_n \\
\Rightarrow \qquad S_n &= 2^{n+1} - 1 && \text{(solution)} \qquad (3.2.2)
\end{aligned}$$

For instance, for $n = 3$, the value of the sum (3.2.1) is

$$2^0 + 2^1 + 2^2 + 2^3 \;=\; 1 + 2 + 4 + 8 \;=\; 15$$

and the value of the closed formula (3.2.2) is

$$2^4 - 1 \;=\; 16 - 1 \;=\; 15$$

A Classical Example of Perturbation

Example 3.2.2: A classic example to show the power of the method of perturbation is the sum

$$S_n \;=\; \sum_{k=0}^{n} k2^k \qquad (3.2.3)$$

which is not so easily evaluated by the most elementary methods. The setup used here (and on Example 3.2.1) is characteristic of applications of the perturbation method.

$$
\begin{aligned}
S_n + (n+1)2^{n+1} &= 0 \cdot 2^0 + \sum_{k=1}^{n+1} k2^k = \sum_{k=1}^{n+1} k2^k && \text{(set up)} \\
&= \sum_{k=0}^{n} (k+1)2^{k+1} && \text{(change of limits)} \\
&= \sum_{k=0}^{n} k2^{k+1} + \sum_{k=0}^{n} 2^{k+1} && \text{(Addition Law)} \\
&= 2\sum_{k=0}^{n} k2^k + 2\sum_{k=0}^{n} 2^k && \text{(Distributive Law)} \\
&= 2S_n + 2(2^{n+1} - 1) && \text{(from Example 3.2.1)} \\
\Rightarrow \qquad S_n &= (n+1)2^{n+1} - 2(2^{n+1} - 1) \\
&= (n-1)2^{n+1} + 2 \qquad \text{(solution)} && (3.2.4)
\end{aligned}
$$

For $n = 3$, the result of the term-by-term summation (3.2.3)

$$
\begin{aligned}
\sum_{k=0}^{3} k2^k &= 0 \cdot 2^0 + 1 \cdot 2^1 + 2 \cdot 2^2 + 3 \cdot 2^3 \\
&= 0 + 2 + 8 + 24 = 34
\end{aligned}
$$

agrees with the evaluation of the formula (3.2.4) derived by perturbation.

$$
\begin{aligned}
(n-1)2^{n+1} &= (3-1)2^4 + 2 \\
&= 2 \cdot 16 + 2 = 32 + 2 = 34
\end{aligned}
$$

Indirect Perturbation

When a first perturbation misses the target, it may help to adjust what is to be perturbed and to try a second time, as indicated by the next example.

Example 3.2.3: We evaluate the sum

$$S_n = \sum_{k=0}^{n} H_k \tag{3.2.5}$$

by perturbation, as in previous examples.

$$\begin{aligned}
S_n + H_{n+1} &= H_0 + \sum_{k=1}^{n+1} H_k = 0 + \sum_{k=1}^{n+1} H_k \\
&= \sum_{k=0}^{n} H_{k+1} = \sum_{k=0}^{n} \left(H_k + \frac{1}{k+1} \right) \\
&= \sum_{k=0}^{n} H_k + \sum_{k=0}^{n} \frac{1}{k+1} \\
&= S_n + \sum_{k=0}^{n} \frac{1}{k+1} \\
\Rightarrow \qquad H_{n+1} &= \sum_{k=0}^{n} \frac{1}{k+1} \qquad (3.2.6)
\end{aligned}$$

Formula (3.2.6) is quite correct, but it is not what was wanted, since the symbol S_n cancelled out. When this occurs, a standard maneuver is to multiply the summand by the index variable k and to perturb the result.

Example 3.2.3, cont.: Multiplying the summand H_k by the index variable in this example yields the summation

$$S_n = \sum_{k=0}^{n} kH_k \qquad (3.2.7)$$

which we now perturb, as follows.

$$\begin{aligned}
S_n + (n+1)H_{n+1} &= 0H_0 + \sum_{k=1}^{n+1} kH_k \\
&= 0 + \sum_{k=1}^{n+1} kH_k \\
&= \sum_{k=0}^{n} (k+1)H_{k+1} \\
&= \sum_{k=0}^{n} (k+1)\left(H_k + \frac{1}{k+1}\right) \\
&= \sum_{k=0}^{n} (k+1)H_k + \sum_{k=0}^{n} \frac{k+1}{k+1} \\
&= \sum_{k=0}^{n} kH_k + \sum_{k=0}^{n} H_k + \sum_{k=0}^{n} 1 \\
&= S_n + \sum_{k=0}^{n} H_k + n+1 \\
\Rightarrow \qquad \sum_{k=0}^{n} H_k &= (n+1)H_{n+1} - (n+1) \qquad (3.2.8)
\end{aligned}$$

This time, the result is a formula (3.2.8) for the sum of consecutive harmonic numbers, the formula we actually want. For $n = 3$, directly adding the harmonic numbers, which are the summands of the sum (3.2.5)

$$\sum_{k=0}^{3} H_k \;=\; 0+\left(\frac{1}{1}\right)+\left(\frac{1}{1}+\frac{1}{2}\right)+\left(\frac{1}{1}+\frac{1}{2}+\frac{1}{3}\right) \;=\; \frac{13}{3}$$

and applying the summation formula (3.2.8)

$$4H_4 - 4 \;=\; 4\cdot\frac{25}{12} - 4 \;=\; \frac{25}{3} - 4 \;=\; \frac{13}{3}$$

yield the same result, thereby illustrating correctness of the formula.

As a second example of indirect perturbation, consider the problem of deriving a formula for summing k^2.

Example 3.2.4: To evaluate the sum

$$S_n \;=\; \sum_{k=0}^{n} k^2 \tag{3.2.9}$$

we start as usual.

$$\begin{aligned} S_n + (n+1)^2 \;&=\; 0^2 + \sum_{k=1}^{n+1} k^2 \;=\; \sum_{k=1}^{n+1} k^2 \\ &=\; \sum_{k=0}^{n} (k+1)^2 \;=\; \sum_{k=0}^{n} (k^2+2k+1) \end{aligned}$$

$$= \sum_{k=0}^{n} k^2 + \sum_{k=0}^{n} 2k + \sum_{k=0}^{n} 1 \qquad \text{(Addition Law)}$$

$$= \sum_{k=0}^{n} k^2 + 2\sum_{k=0}^{n} k + \sum_{k=0}^{n} 1 \quad \text{(Distributive Law)}$$

$$= S_n + 2\sum_{k=0}^{n} k + (n+1)$$

$$\Rightarrow \quad \sum_{k=0}^{n} k = \frac{(n+1)^2 - (n+1)}{2} = \frac{n^2+n}{2} \qquad (3.2.10)$$

Thus, as in Example 3.2.3, direct perturbation has yielded a correct equation that is not the desired result. Seeking to remedy this situation, we once again multiply the summand by the index variable and re-perturb.

Example 3.2.4, cont.: Since perturbing the sum of consecutive values of k^2 just above has yielded an evaluation for the sum of consecutive values of k, it may be less than fully surprising that perturbing the sum of values of k^3 yields a formula for the sum of values of k^2. This time, set

$$S_n = \sum_{k=0}^{n} k^3 \qquad (3.2.11)$$

Then

$$S_n + (n+1)^3 = 0^3 + \sum_{k=1}^{n+1} k^3 = \sum_{k=1}^{n+1} k^3$$

$$
\begin{aligned}
&= \sum_{k=0}^{n} (k+1)^3 \\
&= \sum_{k=0}^{n} (k^3 + 3k^2 + 3k + 1) \\
&= \sum_{k=0}^{n} k^3 \; + \; 3\sum_{k=0}^{n} k^2 \; + \; 3\sum_{k=0}^{n} k \; + \; \sum_{k=0}^{n} 1 \\
&= S_n \; + \; 3\sum_{k=0}^{n} k^2 \; + \; 3\sum_{k=0}^{n} k \; + \; \sum_{k=0}^{n} 1
\end{aligned}
$$

$$
\begin{aligned}
\Rightarrow \quad 3\sum_{k=0}^{n} k^2 &= (n+1)^3 \; - \; 3\sum_{k=0}^{n} k \; - \; \sum_{k=0}^{n} 1 \\
&= (n+1)^3 \; - \; \frac{3n^2+3n}{2} \; - \; (n+1) \\
&= (n+1)^3 \; - \; \frac{3n^2+5n+2}{2} \; = \; \frac{2n^3+3n^2+n}{2}
\end{aligned}
$$

$$
\Rightarrow \quad \sum_{k=0}^{n} k^2 \; = \; \frac{2n^3+3n^2+n}{6} \qquad (3.2.12)
$$

For $n = 3$, the value of the sum (3.2.9)

$$
\begin{aligned}
\sum_{k=0}^{3} k^2 &= 0^2 + 1^2 + 2^2 + 3^2 \\
&= 0 + 1 + 4 + 9 \; = \; 14
\end{aligned}
$$

agrees with the value of formula (3.2.12)

$$
\frac{2n^3+3n^2+n}{6} \; = \; \frac{2\cdot 3^3 + 3\cdot 3^2 + 3}{6} \; = \; \frac{84}{6} \; = \; 14
$$

3.3 SUMMING WITH OGF'S

In this section, it will be seen that most of the sums evaluated in §3.2 could easily be evaluated, alternatively, by using OGFs, as indicated by Theorem 1.7.4 and its corollaries, with the aid of partial fractions, as needed.

REVIEW FROM §1.7:

- **Theorem 1.7.4.** Let $B(z)$ be the OGF for a sequence $\langle b_n \rangle$. Then the OGF for the sequence of partial sums of $\langle b_n \rangle$ is
$$\frac{B(z)}{1-z}$$

- **Cor 1.7.5.** $$\frac{1}{(1-z)^r} = \sum_{n=0}^{\infty} \binom{n+r-1}{r-1} z^n$$

- **Cor 1.7.6.** $$\frac{1}{(1-az)^r} = \sum_{n=0}^{\infty} \binom{n+r-1}{r-1} a^n z^n$$

Revisiting Examples

Example 3.2.1, revisited: We examine how to use generating functions to rederive the summation formula

$$\sum_{k=0}^{n} 2^k = 2^{n+1} - 1$$

for the powers of 2. As first mentioned in §1.7, the OGF for the sequence $\langle b_k = 2^k \rangle$ is

$$B(z) \;=\; \frac{1}{1-2z}$$

By Thm 1.7.4, the OGF for the sequence

$$\left\langle u_n \;=\; \sum_{k=0}^{n} b_k \;=\; \sum_{k=0}^{n} 2^k \;\middle|\; n = 0, 1, \ldots \right\rangle$$

is

$$\begin{aligned} U(z) \;=\; \sum_{n=0}^{\infty} u_n z^n \;&=\; \frac{1}{1-z}\, B(z) \\ &=\; \frac{1}{(1-z)(1-2z)} \end{aligned}$$

By the method of partial fractions (described in §2.3), which here involves the solution of a pair of simultaneous linear equations, it follows that

$$\begin{aligned} \frac{1}{(1-z)(1-2z)} \;&=\; \frac{-1}{(1-z)} + \frac{2}{(1-2z)} \\ &=\; \sum_{n=0}^{\infty} (-1) z^n \;+\; \sum_{n=0}^{\infty} 2 \cdot 2^n z^n \\ &=\; \sum_{n=0}^{\infty} (2^{n+1} - 1) z^n \end{aligned}$$

$$\Rightarrow \quad u_n \;=\; \sum_{k=0}^{n} 2^k \;=\; 2^{n+1} - 1$$

Example 3.2.2, revisited: We now rederive the summation formula

$$\sum_{k=0}^{n} k2^k \;=\; (n-1)2^{n+1} + 2$$

Corollary 1.7.6 provides the formula

$$\frac{1}{(1-az)^r} \;=\; \sum_{n=0}^{\infty} \binom{n+r-1}{r-1} a^n z^n$$

into which the substitutions $a = 2$ and $r = 2$ yield

$$\frac{1}{(1-2z)^2} \;=\; \sum_{n=0}^{\infty} \binom{n+1}{1} 2^n z^n \;=\; \sum_{n=0}^{\infty} (n+1)\, 2^n z^n$$

from which it follows that

$$\frac{2z}{(1-2z)^2} \;=\; \sum_{n=0}^{\infty} (n+1)\, 2^{n+1} z^{n+1} \;=\; \sum_{n=0}^{\infty} n\, 2^n z^n$$

Thus, the OGF for the sequence $\langle b_n = n2^n \rangle$ is

$$B(z) \;=\; \frac{2z}{(1-2z)^2}$$

By Theorem 1.7.4, the OGF for its sequence

$$\left\langle v_n \;=\; \sum_{k=0}^{n} k2^k \;\middle|\; n = 0, 1, \ldots \right\rangle$$

of partial sums is

$$V(z) = \sum_{n=0}^{\infty} v_n z^n = \frac{1}{1-z} B(z)$$
$$= \frac{2z}{(1-z)(1-2z)^2}$$

By partial fractions, which this time requires the solution of three simultaneous linear equations, we have

$$\frac{2z}{(1-z)(1-2z)^2} = \frac{2}{(1-z)} + \frac{8z}{(1-2z)^2} - \frac{2}{(1-2z)^2}$$

Thus, by Corollaries 1.7.5 and 1.7.6, it follows that

$$v_n = \sum_{k=0}^{n} k2^k = 2 + 4n \cdot 2^n - (n+1)2^{n+1}$$
$$= (n-1)2^{n+1} + 2$$

For this example, the previous evaluation by perturbation may seem less effort than the method of generating functions, because of the linear equations and the care needed to apply Corollary 1.7.6 accurately.

Example 3.2.4, revisited: To rederive the summation formula

$$\sum_{k=0}^{n} k^2 = \frac{2n^3 + 3n^2 + n}{6}$$

the method of generating functions is easier than perturbation, since it avoids the false start encountered in perturbation, which is unlikely to be discovered until the late stages. To derive the OGF for the sequence $\langle b_k = k^2 \rangle$ we start with Corollary 1.7.5.

$$\frac{1}{(1-z)^r} = \sum_{n=0}^{\infty} \binom{n+r-1}{r-1} z^n$$

For $r = 3$, this yields

$$\frac{1}{(1-z)^3} = \sum_{n=0}^{\infty} \binom{n+2}{2} z^n$$

Therefore,

$$\frac{z^2}{(1-z)^3} = \sum_{n=0}^{\infty} \binom{n}{2} z^n = \sum_{n=0}^{\infty} \frac{n^2-n}{2} z^n$$

and

$$\frac{z}{(1-z)^3} = \sum_{n=0}^{\infty} \binom{n+1}{2} z^n = \sum_{n=0}^{\infty} \frac{n^2+n}{2} z^n$$

from which it follows that

$$\frac{z^2+z}{(1-z)^3} = \sum_{n=0}^{\infty} n^2 z^n = B(z)$$

By Theorem 1.7.4, the OGF for the sequence

$$\left\langle y_n = \sum_{k=0}^{n} k^2 \;\middle|\; n = 0, 1, \ldots \right\rangle$$

is

$$Y(z) = \sum_{n=0}^{\infty} y_n z^n = \frac{B(z)}{1-z} = \frac{z^2+z}{(1-z)^4}$$

Corollary 1.7.5 with $r = 4$ is

$$\frac{1}{(1-z)^4} = \sum_{n=0}^{\infty} \binom{n+3}{3} z^n$$

Thus,

$$\begin{aligned} Y(z) = \frac{z^2+z}{(1-z)^4} &= \sum_{n=0}^{\infty} \binom{n+3}{3} z^{n+2} + \sum_{n=0}^{\infty} \binom{n+3}{3} z^{n+1} \\ &= \sum_{n=0}^{\infty} \binom{n+1}{3} z^n + \sum_{n=0}^{\infty} z \binom{n+2}{3} z^n \end{aligned}$$

Therefore,

$$\begin{aligned} y_n &= \frac{(n+1)^{\underline{3}}}{6} + \frac{(n+2)^{\underline{3}}}{6} \\ &= \frac{n^3-n}{6} + \frac{n^3+3n^2+2n}{6} \\ &= \frac{2n^3+3n^2+n}{6} \end{aligned}$$

3.4 FINITE CALCULUS

In the Fundamental Theorem of Finite Calculus (Theorem 1.4.3), Part (a) asserts how sums can be evaluated as anti-differences, analogous to way the fundamental theorem of infinitessimal calculus asserts that integrals can be evaluated as anti-derivatives.

REVIEW FROM §1.4:

- Given a function $f : \mathbb{R} \to \mathbb{R}$, the ***difference function*** $\triangle f$ is given by the rule

$$\triangle f(x) \;=\; f(x+1) \;-\; f(x) \tag{3.4.1}$$

- Given a sequence $\langle x_n \rangle$, we define the ***difference sequence*** $\langle \triangle x_n \rangle$ by the rule

$$\triangle x_n \;=\; x_n' \;=\; x_{n+1} \;-\; x_n$$

- **Theorem 1.4.3 [Fundamental Theorem of Finite Calculus].** Let $\langle x_n \rangle$ be any standard sequence. Then

$$(a)\ \sum_{j=0}^{n-1} x_j' \;=\; x_n \;-\; x_0; \qquad (b)\ \left(\sum_{j=0}^{k-1} x_j \right)_n' \;=\; x_n$$

Summing a Polynomial

We recall that the finite calculus formulas for differencing and summing a falling power are directly analogous to the infinitessimal calculus formula for differentiating and integrating an ordinary power.

REVIEW FROM §1.5:

- The n^{th} ***falling power*** function on a real variable x, for any $n \in \mathbb{N}$, is defined by the rule

$$x^{\underline{n}} = \overbrace{x(x-1)\cdots(x-n+1)}^{n \text{ factors}}$$

- **Thm 1.5.1.** For $r \in \mathbb{Z}^+$, we have $\triangle(x^{\underline{r}}) = rx^{\underline{r-1}}$.
- **Cor 1.5.2.** For $r \in \mathbb{N}$, we have $\displaystyle\sum_{k=0}^{n-1} k^{\underline{r}} = \frac{n^{\underline{r+1}}}{r+1}$.

REVIEW FROM §1.6:

- **Thm 1.6.1** Any ordinary power x^n equals a linear combination of falling powers, i.e., in the form

$$x^n = \sum_{r=0}^{n} S_{n,r} x^{\underline{r}}$$

where the coefficients $S_{n,r}$ are called *Stirling numbers of the second kind.*

We will now use the reviewed results to see how finite calculus makes many kinds of summation quite routine.

Example 3.2.4, revisited again: In this chapter, we have already derived the summation formula

$$\sum_{k=0}^{n} k^2 = \frac{2n^3 + 3n^2 + n}{6}$$

first using indirect perturbation, and then again with generating functions. For this derivation, summation calculus is easier yet. With finite calculus, we first express k^2 as a linear combination of falling powers. For monomials of low degree, it is easy enough to calculate the coefficients of the falling powers by *ad hoc* methods.

$$\begin{aligned} k^2 &= S_{2,2}\, k^{\underline{2}} + S_{2,1}\, k^{\underline{1}} \\ &= k^{\underline{2}} + k^{\underline{1}} \end{aligned} \tag{3.4.2}$$

Summing both sides of equation (3.4.2), we obtain

$$\begin{aligned} \sum_{k=0}^{n} k^2 &= \sum_{k=0}^{n} (k^{\underline{2}} + k^{\underline{1}}) \\ &= \sum_{k=0}^{n} k^{\underline{2}} + \sum_{k=0}^{n} k^{\underline{1}} \end{aligned}$$

Applying Corollary 1.5.2 now yields

$$\begin{aligned}\sum_{k=0}^{n} k^2 &= \left.\frac{k^{\underline{3}}}{3}\right|_{k=0}^{n+1} + \left.\frac{k^{\underline{2}}}{2}\right|_{k=0}^{n+1} \\ &= \frac{(n+1)^{\underline{3}}}{3} + \frac{(n+1)^{\underline{2}}}{2} \\ &= \frac{n^3-n}{3} + \frac{n^2+n}{2} \\ &= \frac{2n^3+3n^2+n}{6}\end{aligned}$$

Formula for Summing Exponentials

The supply of useful finite summation formulas is readily extended beyond the monomial formula of Corollary 1.5.2. This begins with sums and differences of exponentiations in which the base is constant and the exponent is variable.

Theorem 3.4.1. *Let the constant value c be a real number and let x be a real or integer variable. Then*

$$\triangle c^x = (c-1)c^x$$

Proof: $\triangle c^x = c^{x+1} - c^x = (c-1)\,c^x.$ ♢

Example 3.4.1: For the case $c = 2$, Theorem 3.4.1 gives the result

$$\triangle 2^x = (2-1)\,2^x = 2^x$$

which is analogous to the differential-calculus result

$$\frac{d}{dx}\, e^x \;=\; e^x$$

This is one of numerous reasons why the number 2 is regarded as the natural base of discrete mathematics in the same sense that the real number e is the natural base for continuous mathematics. More generally, the continuous-mathematics formula

$$\frac{d}{dx}\, c^x \;=\; \ln c \cdot c^x$$

is analogous to the discrete-mathematics formula of Theorem 3.4.1.

$$\triangle c^x \;=\; (c-1)\, c^x$$

Example 3.4.2

$$\begin{aligned} \triangle 3^x &= 3^{x+1} - 3^x = 2 \cdot 3^x \\ \triangle 4^x &= 4^{x+1} - 4^x = 3 \cdot 4^x \end{aligned}$$

This leads to a major formula of the finite-summation calculus, the formula for summing exponentials.

Corollary 3.4.2 [Exponential Formula]. *Let c be any real number except 1. Then*

$$\sum_{k=0}^{n-1} c^k \;=\; \frac{c^n - 1}{c - 1} \qquad (3.4.3)$$

Proof: For $c \neq 1$, applying the Fundamental Theorem of Finite Calculus to the conclusion of Theorem 3.4.1 implies that

$$\sum_{k=0}^{n-1} c^k = \left.\frac{c^k}{c-1}\right|_{k=0}^{n} = \frac{c^n - 1}{c-1} \qquad \diamondsuit$$

Remark: For the case $c = 1$, which is excluded from Corollary 3.4.2, we have the sum

$$\sum_{k=0}^{n-1} 1^k = n$$

Example 3.4.3: We observe that when $c = 5$ and $n = 4$, the value of the sum on the left side of equation (3.4.3)

$$\sum_{k=0}^{3} 5^k = 5^0 + 5^1 + 5^2 + 5^3 = 1 + 5 + 25 + 125 = 156$$

agrees with the value of the quotient on the right side

$$\frac{5^4 - 1}{4} = \frac{625 - 1}{4} = 156$$

As easy as it was to derive the formula

$$\sum_{k=0}^{n} 2^k = 2^{n+1} - 1$$

either with perturbation or with generating functions, it is even easier with the calculus of summation, as now shown.

Example 3.2.1, revisited again: According to Theorem 3.4.1, we have

$$\triangle 2^k = 2^k$$

Summing both sides, we obtain

$$\sum_{k=0}^{n} 2^k = \sum_{k=0}^{n} \triangle 2^k$$

after which, applying the Fundamental Theorem yields the result

$$\begin{aligned} \sum_{k=0}^{n} 2^k &= 2^k \Big|_{k=0}^{n+1} \\ &= 2^{n+1} - 1 \end{aligned}$$

Falling Negative Powers

The extension of the list of useful differencing and summation formulas continues. We observe that nonnegative falling powers can be defined recursively.

$$\begin{aligned} x^{\underline{0}} &= 1 \\ x^{\underline{r+1}} &= x^{\underline{r}}(x - r) \qquad \text{for } r > 0 \end{aligned}$$

Running the recursion backward extends the utility of the falling power concept.

DEF: ***Non-positive falling powers*** are defined as follows.

$$x^{\underline{0}} = 1$$
$$x^{\underline{r}} = \frac{x^{\underline{r+1}}}{x-r} \qquad \text{for } r < 0$$

Example 3.4.4: Here are a few evaluations of the definition of negative falling powers.

$$x^{\underline{-1}} = \frac{x^{\underline{0}}}{x-(-1)} = \frac{x^{\underline{0}}}{x+1} = \frac{1}{x+1}$$
$$x^{\underline{-2}} = \frac{x^{\underline{-1}}}{x-(-2)} = \frac{x^{\underline{-1}}}{x+2} = \frac{1}{(x+1)(x+2)}$$
$$x^{\underline{-3}} = \frac{x^{\underline{-2}}}{x-(-3)} = \frac{x^{\underline{-2}}}{x+3} = \frac{1}{(x+1)(x+2)(x+3)}$$

Proposition 3.4.3. *For any positive number r and any real number x,*

$$x^{\underline{-r}} = \frac{1}{(x+1)\cdots(x+r)}$$

Proof: By induction on r. ♢

Although ordinary powers are additive in a product of ordinary monomials with the same base, in the sense that

$$x^r \cdot x^s = x^{r+s}$$

it is clear that falling powers are not additive in a product of falling-power monomials. For instance,

$$x^{\underline{2}} \cdot x^{\underline{3}} \;=\; x(x-1)\cdot x(x-1)(x-2)$$

but

$$x^{\underline{2+3}} \;=\; x^{\underline{5}} \;=\; x(x-1)(x-2)(x-3)(x-4)$$

Thus, there is no reason to expect that $x^{\underline{-r}} = (x^{\underline{r}})^{-1}$. On the other hand, an important analogy to infinitessimal calculus is preserved.

Proposition 3.4.4. *The difference formula for negative falling powers is the same formula as for positive falling powers. That is, for every positive integer* r,

$$\triangle x^{\underline{-r}} \;=\; (-r)x^{\underline{-r-1}}$$

Proof: Start by applying the defining formula (3.4.1) for the difference operator.

$$\begin{aligned}\triangle x^{\underline{-r}} &= (x+1)^{\underline{-r}} - x^{\underline{-r}} \\ &= \frac{1}{(x+2)\cdots(x+r+1)} - \frac{1}{(x+1)\cdots(x+r)}\end{aligned}$$

Then by routine manipulation

$$\begin{aligned} &= \frac{1}{(x+2)\cdots(x+r)}\left[\frac{1}{x+r+1} - \frac{1}{x+1}\right] \\ &= \frac{1}{(x+2)\cdots(x+r)}\left[\frac{-r}{(x+1)(x+r+1)}\right]\end{aligned}$$

$$= \frac{-r}{(x+1)\cdots(x+r+1)}$$

we achieve the result

$$\triangle x^{\underline{-r}} = (-r)x^{\underline{-r-1}} \qquad \diamondsuit$$

Cor 3.4.5. *For any integer $r \neq 0$ and any real number x,*

$$\triangle x^{\underline{r}} = rx^{\underline{r-1}}$$

Proof: This combines Thm 1.5.1 and Prop 3.4.4. ♢

Cor 3.4.6 [Monomial Formula]. *For integers $r \neq -1$ and n,*

$$\sum_{k=0}^{n-1} k^{\underline{r}} = \left.\frac{k^{\underline{r+1}}}{r+1}\right|_{k=0}^{n} \qquad (3.4.4)$$

Proof: This combines the Fundamental Theorem and Corollary 3.4.5. ♢

Example 3.4.5: To make a direct evaluation of the left side of Equation (3.4.4) for $r = -2, -3$ and $n = 4$, we first calculate the following partial table of the values of $k^{\underline{r}}$, i.e., of a small integer to a small falling negative power.

r	$0^{\underline{r}}$	$1^{\underline{r}}$	$2^{\underline{r}}$	$3^{\underline{r}}$	$4^{\underline{r}}$	$\cdots$
-1	$\frac{1}{1}$	$\frac{1}{2}$	$\frac{1}{3}$	$\frac{1}{4}$	$\frac{1}{5}$	$\cdots$
-2	$\frac{1}{1\cdot 2}$	$\frac{1}{2\cdot 3}$	$\frac{1}{3\cdot 4}$	$\frac{1}{4\cdot 5}$	$\frac{1}{5\cdot 6}$	$\cdots$
-3	$\frac{1}{1\cdot 2\cdot 3}$	$\frac{1}{2\cdot 3\cdot 4}$	$\frac{1}{3\cdot 4\cdot 5}$	$\frac{1}{4\cdot 5\cdot 6}$	$\frac{1}{5\cdot 6\cdot 7}$	$\cdots$

Case $\mathbf{r = -2}$ and $\mathbf{n = 4}$: The value on the left side is

$$0^{\underline{-2}} + 1^{\underline{-2}} + 2^{\underline{-2}} + 3^{\underline{-2}} = \frac{1}{1\cdot 2} + \frac{1}{2\cdot 3} + \frac{1}{3\cdot 4} + \frac{1}{4\cdot 5} = \frac{4}{5}$$

and the value on the right side is

$$\left.\frac{k^{\underline{-1}}}{-1}\right|_{k=0}^{4} = \frac{4^{\underline{-1}}}{-1} - \frac{0^{\underline{-1}}}{-1} = \frac{1}{(-1)\cdot 5} - \frac{1}{-1} = \frac{-1}{5} - (-1) = \frac{4}{5}$$

Case $\mathbf{r = -3}$ and $\mathbf{n = 4}$: The value on the left side is

$$0^{\underline{-3}} + 1^{\underline{-3}} + 2^{\underline{-3}} + 3^{\underline{-3}} =$$
$$\frac{1}{1\cdot 2\cdot 3} + \frac{1}{2\cdot 3\cdot 4} + \frac{1}{3\cdot 4\cdot 5} + \frac{1}{4\cdot 5\cdot 6} = \frac{7}{30}$$

and the value on the right side is

$$\left.\frac{k^{\underline{-2}}}{-2}\right|_{k=0}^{4} = \frac{4^{\underline{-2}}}{-2} - \frac{0^{\underline{-2}}}{-2} = \frac{1}{(-2)\cdot 5\cdot 6} - \frac{1}{(-2)\cdot 1\cdot 2} = \frac{7}{30}$$

Harmonic Numbers

Another analogy between the natural logarithm $\ln n$ and the harmonic number H_n lies in the similarity of the derivative

$$\frac{d}{dx}\ln x = x^{-1}$$

to the difference formula

$$\begin{aligned}\triangle H_n &= H_{n+1} - H_n \\ &= \left(\frac{1}{1} + \cdots + \frac{1}{n+1}\right) - \left(\frac{1}{1} + \cdots + \frac{1}{n}\right) \\ &= \frac{1}{n+1} = n^{\underline{-1}}\end{aligned}$$

and, naturally enough, in the similarity of the summation formula

$$\sum_{k=0}^{n-1} k^{\underline{-1}} \;=\; H_n \qquad (3.4.5)$$

to the integration formula

$$\int_{x=1}^{t} x^{-1} dx \;=\; \ln x$$

Product Formula

Analogous to the product formula for derivatives,

$$(u(x) \cdot v(x))' \;=\; u'(x) \cdot v(x) \;+\; u(x) \cdot v'(x)$$

there is a product formula for finite differences.

Prop 3.4.7 [Product Formula]. *Let* $h(x) = g(x) \cdot f(x)$. *Then*

$$\triangle h(x) \;=\; \triangle g(x) \cdot f(x+1) \;+\; g(x) \cdot \triangle f(x) \qquad (3.4.6)$$

Proof: Once again, it is sufficient to do some routine algebraic manipulation, starting from an application of the definition of the difference operator.

$$\begin{aligned} \triangle h(x) &= h(x+1) \;-\; h(x) \\ &= g(x+1) \cdot f(x+1) \;-\; g(x) \cdot f(x) \\ &= g(x+1) \cdot f(x+1) \;-\; g(x) \cdot f(x) \\ &\qquad - g(x) \cdot f(x+1) \;+\; g(x) \cdot f(x+1) \\ &= \triangle g(x) \cdot f(x+1) \;+\; g(x) \cdot \triangle f(x) \end{aligned}$$

♢

Example 3.4.6: Take $g(n) = n^{\underline{2}}$ and $f(n) = H_n$. According to the product formula (3.4.6), we have

$$\begin{aligned}
\triangle(n^{\underline{2}} H_n) &= \triangle n^{\underline{2}} \cdot H_{n+1} \;+\; n^{\underline{2}} \cdot \triangle H_n \\
&= 2n \cdot H_{n+1} \;+\; n(n-1) \cdot \frac{1}{n+1} \\
&= 2n\left(H_n + \frac{1}{n+1}\right) \;+\; \frac{n^2 - n}{n+1} \\
&= 2nH_n \;+\; \frac{n^2 + n}{n+1} \\
&= 2nH_n \;+\; n
\end{aligned}$$

Unsurprisingly, evaluating the defining formula (3.4.1) for a finite difference yields the identical result.

$$\begin{aligned}
\triangle(n^{\underline{2}} H_n) &= (n+1)^{\underline{2}} H_{n+1} \;-\; n^{\underline{2}} H_n \\
&= (n^2 + n)\left(H_n + \frac{1}{n+1}\right) \;-\; (n^2 - n)H_n \\
&= (n^2 + n)H_n + \frac{n^2 + n}{n+1} \;-\; (n^2 - n)H_n \\
&= 2n\, H_n \;+\; n
\end{aligned}$$

Summation by Parts

From the infinitessimal calculus, we recall the following formula for integration by parts

$$\int_a^b u(x)v'(x)dx \;=\; u(x)v(x)\Big|_a^b \;-\; \int_a^b u'(x)v(x)dx$$

The finite calculus has an analogous formula, called *summation by parts.*

Proposition 3.4.8 [Summation by Parts]. *Let $g(k)$ and $f(k)$ be functions on the integers. Then*

$$\sum_{k=0}^{n-1} g(k) \triangle (f(k)) \;=\; g(k) f(k) \Big|_{k=0}^{n} - \sum_{k=0}^{n-1} \triangle(g(k))\, f(k+1) \tag{3.4.7}$$

Proof: This corollary to Proposition 3.4.7 follows from the Fundamental Theorem of Finite Calculus. ◇

Example 3.2.2, revisited again: After using the substitutions

$$g(k) \;=\; k^{\underline{1}} \qquad \text{and} \qquad f(k) \;=\; 2^k$$

summing the sequence $\langle k2^k \mid k = 0,\ 1,\ 2,\ \ldots \rangle$ by parts takes the form

$$\begin{aligned} \sum_{k=0}^{n} k2^k \;&=\; \sum_{k=0}^{n} k^{\underline{1}}\, 2^k \\ &=\; k^{\underline{1}}\, 2^k \Big|_{0}^{n+1} - \sum_{k=0}^{n} k^{\underline{0}}\, 2^{k+1} \end{aligned}$$

which leads to the calculations

$$\begin{aligned} &=\; (n+1) \cdot 2^{n+1} \;-\; 2\sum_{k=0}^{n} 2^k \\ &=\; (n+1) \cdot 2^{n+1} \;-\; 2(2^{n+1} - 1) \\ &=\; (n-1) \cdot 2^{n+1} \;+\; 2 \end{aligned}$$

Example 3.2.3, revisited: Since integration by parts is helpful in evaluating the integral of $\ln x$ to $x \ln x - x$, it is unsurprising that summation by parts is helpful in summing H_n to $nH_n - n$.

$$\begin{aligned}
\sum_{k=0}^{n-1} H_k &= \sum_{k=0}^{n-1} k^{\underline{0}} H_k \\
&= k^{\underline{1}} H_k \Big|_0^n - \sum_{k=0}^{n-1} (k+1)^{\underline{1}} \frac{1}{k+1} = k^{\underline{1}} H_k \Big|_0^n - \sum_{k=0}^{n-1} 1 \\
&= (nH_n - 0) - n \\
&= nH_n - n
\end{aligned}$$

Table 3.4.1 Formulas for the calculus of differences.

function	difference function
$k^{\underline{r}}$	$r\,k^{\underline{r-1}}$
c^k	$(c-1)\,c^k$
H_n	$\dfrac{1}{n+1}$
$g(k)f(k)$	$\triangle g(x)\,f(x+1) + g(x)\,\triangle f(x)$

Table 3.4.2 **Formulas for finite summations.**

summation	formula	reference
$\sum_{k=0}^{n-1} c^k, \quad c \neq 0$	$\frac{c^n - 1}{c - 1}$	(3.4.3)
$\sum_{k=0}^{n-1} k^{\underline{r}}, \quad r \neq -1$	$\frac{n^{\underline{r+1}}}{r+1}$	(3.4.4)
$\sum_{k=0}^{n-1} k^{\underline{-1}}$	H_n	(3.4.5)
$\sum_{k=0}^{n-1} g(k) \triangle (f(k))$	$g(k)f(k)\Big\vert_{k=0}^{n} - \sum_{k=0}^{n-1} \triangle(g(k))\, f(k+1)$	(3.4.7)

3.5 ITERATED SUMS

In the simplest case of iterated summation the index set U

$$S = \sum_{i \in U} x_i$$

is a 2-dimensional array, such that one could first take the row sums and then add those sums to get the total. Sometimes the first summation, called the *inner summation*, is for groupings other than rows. Sometimes, when given a double summation to evaluate, it is helpful to swap the order of summation.

Double summation need not be twice as hard. Indeed, sometimes a single sum is recast as a double sum to make it more tractable. A possible strategy in evaluating a difficult sum

$$S = \sum_{i \in U} x_i$$

is to find a partition

$$U = \bigcup_{k \in K} U_k$$

such that each of the sub-sums

$$S_k = \sum_{i \in U_k} x_i$$

is tractable, and also such that the sum

$$\sum_{k \in K} S_k = \sum_{k \in K} \sum_{i \in U_k} x_i$$

of the sub-sums is tractable.

Independent Indices

An example from graph theory illustrates the simplest case of a double summation, in which the index of the inner sum is independent of the index of the outer sum.

Example 3.5.1: The degree of a vertex v of a graph is the total number of edge-incidences on v. Each edge e contributes 0, 1, or 2 to that total, corresponding to the number $I(v, e)$ of times that vertex v is an endpoint of edge e. Figure 3.5.1 shows a graph, with its vertex degrees as bold numbers.

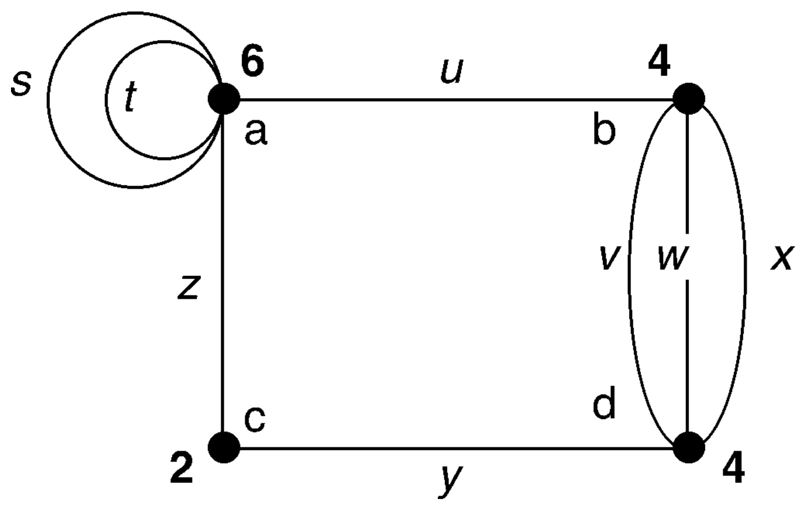

Fig 3.5.1 **Degrees of the vertices of a graph.**

Thus, the sum of all the edge-vertex incidences

$$\sum_{(v,e)\,\in V\times E} I(v,e)$$

is indexed by the cartesian product $V \times E$, where V is the set of vertices and E the set of edges. The obvious partition of this sum over a cartesian product of two sets is into an iterated sum

$$\sum_{(v,e)\,\in V\times E} I(v,e) \;=\; \sum_{v\in V}\sum_{e\in E} I(v,e)$$

over the incidence matrix, with rows labeled by vertices and columns by edges, so that the row-sums are the degrees.

	s	t	u	v	v	x	y	z	degree
a	2	2	1	0	0	0	0	1	6
b	0	0	1	1	1	1	0	0	4
c	0	0	0	0	0	0	1	1	2
d	0	0	0	1	1	1	1	0	4

Of course, the result of adding the row-sums of an array equals the result of adding the column-sums. In this case, since every column-sum is 2, adding the column-sums is equivalent to doubling the number of edges, which is faster than adding degree-sums. This observation yields an alternative proof of Euler's Degree-Sum Theorem (Theorem 0.6.1).

Thm 3.5.1 [Euler's Degree-Sum Thm]. *The sum of the degrees of the vertices of a graph equals twice the number of edges.*

Proof: Let $V = (V, E)$ be a graph. Then starting from row sums

$$\sum_{v \in V} \deg(v) = \sum_{v \in V} \sum_{e \in E} I(v, e) \qquad \text{sum of row sums}$$

swap the order of summation:

$$\begin{aligned} &= \sum_{e \in E} \sum_{v \in V} I(v, e) && \text{sum of column sums} \\ &= \sum_{e \in E} 2 && \text{every column sum is 2} \\ &= 2\,|E| && \diamondsuit \end{aligned}$$

Interchanging the order of summation is a fundamental technique for evaluating an iterated sum over an array. It is useful when the implicit repartitioning yields inner sums and an outer sum for which the total effort of evaluation is less than that for the given iterated summation problem.

In this instance, the cost of repartitioning was trivial, because the index of the inner sum of the given iterated sum was *independent* of the index of the outer sum.

Dependent Indices

If the limits of the index of the inner sum are independent of the index of the outer sum, then the order of summation can be transposed without changing the limits of either index. However, it is quite common for the outer index to range from 1 to n, while the upper limit of the inner index equals the outer index. As illustrated in Figure 3.5.2, this amounts to summing over the rows of the lower-left triangle of an $n \times n$ array.

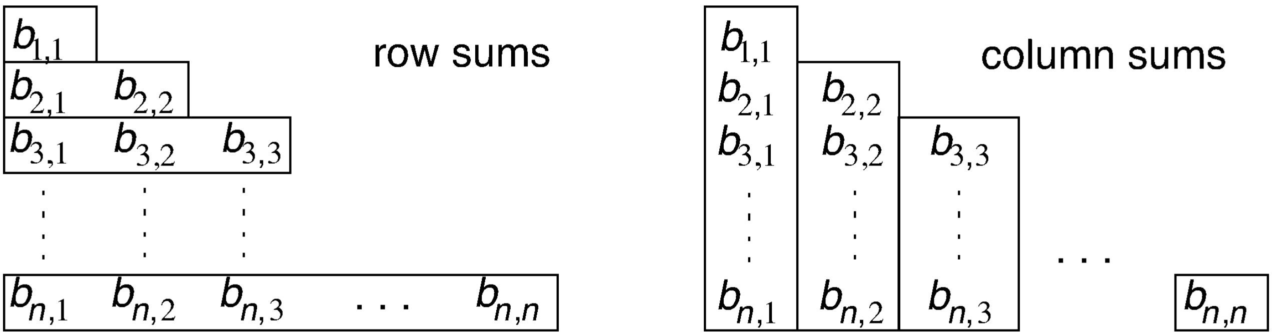

Fig 3.5.2 Row sums and column sums.

Interchanging the order of summation for this form of iterated sum turns the outer sums into column sum. The new inner index (the row index) has the outer index (the column index) as its lower limit and ranges up to n.

Example 3.2.3, revisited: The sum of the harmonic numbers has previously been evaluated by perturbation and by finite calculus. Another effective method is going to a double sum and then interchanging the order of summation.

$$
\begin{aligned}
\sum_{k=0}^{n-1} H_k &= \sum_{k=0}^{n-1} \sum_{j=1}^{k} \frac{1}{j} && \text{write as double sum} \\
&= \sum_{j=1}^{n-1} \sum_{k=j}^{n-1} \frac{1}{j} && \text{swap order of summation} \\
&= \sum_{j=1}^{n-1} \frac{1}{j} \sum_{k=j}^{n-1} 1 && \text{factor out constant} \\
&= \sum_{j=1}^{n-1} \frac{1}{j} (n-j) && \text{evaluate inner sum} \\
&= \sum_{j=1}^{n-1} \left(\frac{n}{j} - \frac{j}{j} \right) \\
&= \sum_{j=1}^{n} \left(\frac{n}{j} - \frac{j}{j} \right) && \text{add zero} \\
&= \sum_{j=1}^{n} \frac{n}{j} - \sum_{j=1}^{n} \frac{j}{j} \quad = \quad n \sum_{j=1}^{n} \frac{1}{j} - \sum_{j=1}^{n} 1 \\
&= nH_n - n
\end{aligned}
$$

In circumstances when swapping rows and columns of an array does not adequately reduce the evaluation, it may help to reorganize the partitioning of summation so that the inner sum is over some tractable geometric pattern other than a row or column.

Example 3.5.2: To envision how to repartition the double sum

$$\sum_{k=1}^{n}\sum_{j=1}^{k-1}\frac{1}{k-j}$$

as an aid in evaluation, it helps to write out the array of summands, like this.

$k\downarrow$	1	2	3	4	$j\rightarrow$
2	$\frac{1}{1}$				
3	$\frac{1}{2}$	$\frac{1}{1}$			
4	$\frac{1}{3}$	$\frac{1}{2}$	$\frac{1}{1}$		
5	$\frac{1}{4}$	$\frac{1}{3}$	$\frac{1}{2}$	$\frac{1}{1}$	

Evidently, summing rows or columns amounts to summing the harmonic numbers. However, the strategy of summing on the southeastward diagonals (in which the entries are constant) yields the following result, which is consistent with Example 3.2.3, which also sums harmonic numbers.

$$\begin{aligned}\sum_{d=1}^{n}\sum_{j=1}^{n-d}\frac{1}{d} &= \sum_{d=1}^{n}\frac{n-d}{d} = \sum_{d=1}^{n}\frac{n}{d} - \sum_{d=1}^{n}\frac{d}{d}\\ &= n\sum_{d=1}^{n}\frac{1}{d} - \sum_{d=1}^{n}1 = nH_n - n\end{aligned}$$

Linear Partitioning: Floor Sums

Sometimes a sequence of less tractable summands can be partitioned into consecutive finite subsequences with tractable sums. In particular, this may occur when the summands are the floors or ceilings of a non-decreasing sequence.

Example 3.5.3: Seeking to evaluate a sum of floors may suggest resorting to an approximation, such as

$$\begin{aligned}\sum_{k=0}^{n} \left\lfloor \sqrt{k} \right\rfloor &\approx \sum_{k=0}^{n} \sqrt{k} \\ &\approx \int_{x=0}^{n} x^{1/2} dx \\ &= \frac{2}{3} x^{3/2} \Big|_{x=0}^{n} \\ &= \frac{2}{3} n^{3/2}\end{aligned}$$

For $n = 9$, the value of this approximation is

$$\frac{2}{3} n^{3/2} \Big|_{n=9} = \frac{2}{3} \cdot 9^{3/2} = \frac{2}{3} \cdot 27 = 18$$

whereas the exact value is

$$\begin{aligned}&\left\lfloor \sqrt{0} \right\rfloor + \left\lfloor \sqrt{1} \right\rfloor + \left\lfloor \sqrt{2} \right\rfloor + \left\lfloor \sqrt{3} \right\rfloor \\ &\qquad + \left\lfloor \sqrt{4} \right\rfloor + \left\lfloor \sqrt{5} \right\rfloor + \left\lfloor \sqrt{6} \right\rfloor + \left\lfloor \sqrt{7} \right\rfloor + \left\lfloor \sqrt{8} \right\rfloor + \left\lfloor \sqrt{9} \right\rfloor \\ &= 0 + 1 + 1 + 1 + 2 + 2 + 2 + 2 + 2 + 3 = 16\end{aligned}$$

Sometimes, an approximation this rough meets the purpose at hand. However, it is helpful to be in command of methods that get an exact value when it is needed. There are five steps in the derivation of an exact evaluation formula for such a sum by the method of linear partitioning.

Step 1. List the early terms of the sequence, and partition them according to the value of the summand.

Step 2. Express the size of all but the last cell.

Step 3. Express the size of the last cell, which needs individual attention, since its size might not follow the same rule as the other cells.

Step 4. Evaluate the given sum.

Step 5. Confirm for a small case.

We now demonstrate the application of this method to Example 3.5.3.

Example 3.5.3, cont.: As the index k of the sum

$$\sum_{k=0}^{n} \left\lfloor \sqrt{k} \right\rfloor$$

increases, the value of the summand $\lfloor k \rfloor$ increases also, but more slowly than the index itself.

Step 1 is to partition the index values according to the value of the summand. The partition for $k = 0, 1, \ldots 17$ is as follows:

Table 3.5.1 **Partitioning for the summand $\lfloor k \rfloor$.**

	1		3				5					7					
k	0	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17
$\lfloor \sqrt{k} \rfloor$	0	1	1	1	2	2	2	2	2	3	3	3	3	3	3	3	4	4

Step 2 is to express the sizes of all but the last cell. Each other cell in Table 3.5.1 is grouped with an overbrace, with its size written over the overbrace. The smallest number within each cell is the square m^2 of some number m. Since the number $(m+1)^2$ starts the next cell, it follows that the cell containing m^2 is

$$\{m^2,\ m^2+1,\ \ldots,\ m^2+2m\}$$

Evidently,

$$\#\,\{m^2,\ m^2+1,\ \ldots,\ m^2+2m\} \;=\; 2m+1$$

Step 3 is to express the size of the last cell

$$\{ \lfloor\sqrt{n}\,\rfloor^2, \; \ldots, \; n\}$$

whose entries correspond to the uppermost summand $\lfloor\sqrt{n}\,\rfloor$. $\blacksquare$
Its size is

$$\#\{ \lfloor\sqrt{n}\,\rfloor^2, \; \ldots, \; n\} \;=\; n - \lfloor\sqrt{n}\,\rfloor^2 + 1$$

Step 4. To evaluate the given sum, we multiply each of the realized values of the summand by the corresponding number of values of the index k and then sum the products.

$$\begin{aligned}
\sum_{k=0}^{n} \lfloor\sqrt{k}\,\rfloor \;&=\; \sum_{m=0}^{\lfloor\sqrt{n}\,\rfloor-1} (2m+1)\cdot m \;+\; \left(n - \lfloor\sqrt{n}\,\rfloor^2 + 1\right)\cdot\lfloor\sqrt{n}\rfloor \\
&=\; \sum_{m=0}^{\lfloor\sqrt{n}\rfloor-1} \left(2m^{\underline{2}} + 3m^{\underline{1}}\right) \;+\; \left(n - \lfloor\sqrt{n}\,\rfloor^2 + 1\right)\cdot\lfloor\sqrt{n}\rfloor \\
&=\; \left(\frac{2m^{\underline{3}}}{3} + \frac{3m^{\underline{2}}}{2}\right)\Bigg|_{m=0}^{\lfloor\sqrt{n}\rfloor} \;+\; \left(n - \lfloor\sqrt{n}\rfloor^2 + 1\right)\cdot\lfloor\sqrt{n}\rfloor \\
&=\; \frac{2\lfloor\sqrt{n}\rfloor^{\underline{3}}}{3} + \frac{3\lfloor\sqrt{n}\rfloor^{\underline{2}}}{2} \;+\; \left(n - \lfloor\sqrt{n}\rfloor^2 + 1\right)\cdot\lfloor\sqrt{n}\rfloor
\end{aligned}$$

Step 5. We confirm for the small case $n = 11$.
Sum values in Step 1:

$$0+1+1+1+2+2+2+2+2+3+3+3 = 22$$

Compare with the value by formula of Step 4.

$$\frac{2\lfloor\sqrt{11}\rfloor^3}{3} + \frac{3\lfloor\sqrt{11}\rfloor^2}{2} + \left(11 - \left\lfloor\sqrt{11}\right\rfloor^2 + 1\right)\cdot\left\lfloor\sqrt{11}\right\rfloor$$
$$= 4 + 9 + 3\cdot 3 = 22$$

Example 3.5.4: We now use linear partitioning to evaluate the sum

$$\sum_{k=1}^{n} \lfloor \lg k \rfloor$$

Step 1. List the early terms of the sequence, and partition them according to the value of the summand.

$$\begin{array}{c|cccccccccccccccc} & \overbrace{\ }^{1} & \overbrace{\ \ }^{2} & & \overbrace{\ \ \ \ }^{4} & & & \overbrace{\ \ \ \ }^{8} & & \overbrace{\ \ \ \ }^{16} & & & & & \\ k & 1 & 2\ 3 & 4 & 5\ 6 & 7 & 8 \cdots 15 & 16 \cdots 31 & 32 & 33 & \cdots \\ \lfloor \lg k \rfloor & 0 & 1\ 1 & 2 & 2\ 2 & 2 & 3 \cdots 3 & 4 \cdots 4 & 5 & 5 & \cdots \end{array}$$

Step 2. To express the size of all but the last cell, we observe that the cell corresponding to the summand m is

$$\{2^m,\ 2^m+1,\ \ldots,\ 2^{m+1}-1\}$$

Its size is

$$\#\{2^m,\ 2^m+1,\ \ldots,\ 2^{m+1}-1\} = 2^m$$

Step 3. The last cell is

$$\left\{2^{\lfloor \lg n \rfloor},\ 2^{\lfloor \lg n \rfloor}+1,\ \ldots,\ n\right\}$$

Its size is

$$n - 2^{\lfloor \lg n \rfloor} + 1$$

Step 4. Evaluate the given sum, using the previously derived formula (e.g., see Example 3.2.2) for summing $k \cdot 2^k$.

$$\begin{aligned} \sum_{k=1}^{n} \lfloor \lg k \rfloor &= \sum_{m=1}^{\lfloor \lg n \rfloor - 1} m \cdot 2^m \ + \ \lfloor \lg n \rfloor \left(n - 2^{\lfloor \lg n \rfloor} + 1 \right) \\ &= \left(\lfloor \lg n \rfloor - 2 \right) \cdot 2^{\lfloor \lg n \rfloor} \ + \ 2 \ + \ \lfloor \lg n \rfloor \left(n - 2^{\lfloor \lg n \rfloor} + 1 \right) \end{aligned}$$

Step 5. Confirm for the small case $n = 9$.
Sum the values in Step 1: $0+1+1+2+2+2+2+3+3 = 16$.
Compare with the value given by the formula of Step 4.

$$\begin{aligned} & \left(\lfloor \lg 9 \rfloor - 2 \right) \cdot 2^{\lfloor \lg 9 \rfloor} \ + \ 2 \ + \ \lfloor \lg 9 \rfloor \left(n - 2^{\lfloor \lg 9 \rfloor} + 1 \right) \\ = \ & (3 - 2) \cdot 2^3 \ + \ 2 \ + \ 3(9 - 2^3 + 1) \\ = \ & 1 \cdot 2^3 \ + \ 2 \ + \ 3 \cdot 2 \ = \ 16 \end{aligned}$$

Remark: The two evaluations just considered have an easy second step, because within each group the value of the summand is constant. If the summand were $k\lfloor\sqrt{k}\rfloor$, for instance, then an inner sum might be introduced in Step 2 for the partial sum over the interval corresponding to a group.

3.6 INCLUSION-EXCLUSION

Sometimes, the index set for a complicated sum has subsets with tractable sums, but those subsets overlap. The strategic insight of the inclusion-exclusion method is that the partial sums over those subsets can be combined into a total sum by subtracting the overcounts.

Venn Diagrams for Overlapping Subsets

The simplest case has two overlapping subsets, A and B, as in Figure 3.6.1. The domain from which both subsets are drawn is denoted U.

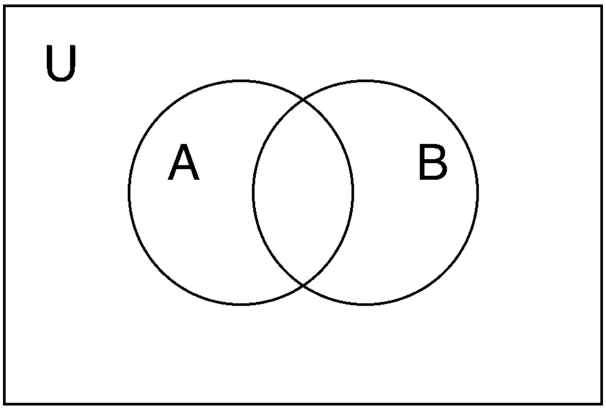

Fig 3.6.1 Venn diagram for two overlapping subsets.

Suppose that the objective is to calculate the sum $S_{A \cup B}$ over the set $A \cup B$, with partial sums S_A, S_B, and $S_{A \cap B}$ over subsets A, B, and $S_{A \cap B}$, respectively. Then

$$S_{A \cup B} \;=\; S_A + S_B - S_{A \cap B}$$

Example 3.6.1: The number of integers in the range $1, \ldots, n$ that are divisible either by 2 or by 3 is expressible as a consecutive sum with indexing in the integer interval $[1 : n]$ and the summand

$$f(k) \;=\; \begin{cases} 1 & \text{if } n \text{ is divisible either by 2 or by 3} \\ 0 & \text{otherwise} \end{cases}$$

that is, by the sum

$$\sum_{k=1}^{n} (2\backslash k \;\vee\; 3\backslash k)$$

Every number that contributes 1 to this sum lies either in the set $\{k \in [1 : n] \mid 2\backslash k\}$, with cardinality $\lfloor n/2 \rfloor$, or in the set $\{k \in [1 : n] \mid 3\backslash k\}$, with cardinality $\lfloor n/3 \rfloor$. Adding these two cardinalities overcounts by $\lfloor n/6 \rfloor$, the number of integers in $[1 : n]$ that are divisible both by 2 and by 3. Thus,

$$\sum_{k=1}^{n} (2\backslash k \;\vee\; 3\backslash k) \;=\; \left\lfloor \frac{n}{2} \right\rfloor + \left\lfloor \frac{n}{3} \right\rfloor - \left\lfloor \frac{n}{6} \right\rfloor$$

In Figure 3.6.1,

$$A \;=\; \{k \in [1 : n] \mid 2\backslash k\}$$

and

$$B \;=\; \{k \in [1 : n] \mid 3\backslash k\}$$

Their intersection is

$$A \cap B = \{k \in [1:n] \mid 6 \backslash k\}$$

and

$$U = [1:n]$$

In Example 3.6.1, the implicit summand is the number 1, since we counted the number of elements in a set. That is,

$$S_X = \sum_{k \in X} 1 = |X|$$
$$\text{for } X = A,\ B,\ A \cap B, \text{ or } A \cup B$$

Example 3.6.2: A related problem is to calculate the sum of the numbers that are divisible by 2 or 3. Then, instead of having a constant value of 1, the value of the summand equals the index itself. That is,

$$S_X = \sum_{k \in X} k$$
$$\text{for } X = A,\ B\ , A \cap B, \text{ or } A \cup B$$

Thus,

$$S_A = \sum_{2 \,\backslash\, k \leq n} k = \sum_{j=1}^{\lfloor n/2 \rfloor} 2j = 2 \sum_{j=1}^{\lfloor n/2 \rfloor} j = 2\, \frac{\lfloor n/2 \rfloor^2 + \lfloor n/2 \rfloor}{2}$$

Similarly,

$$S_B \;=\; \sum_{3\,\backslash\, k \le n} k \;=\; 3\,\frac{\lfloor n/3 \rfloor^2 + \lfloor n/3 \rfloor}{2}$$

and

$$S_{A\cap B} \;=\; \sum_{6\,\backslash\, k \le n} k \;=\; 6\,\frac{\lfloor n/6 \rfloor^2 + \lfloor n/6 \rfloor}{2}$$

Therefore,

$$\begin{aligned} S_{A\cup B} &= S_a + S_B - S_{A\cap B} \\ &= 2\,\frac{\lfloor n/2 \rfloor^2 + \lfloor n/2 \rfloor}{2} + 3\,\frac{\lfloor n/3 \rfloor^2 + \lfloor n/3 \rfloor}{2} - 6\,\frac{\lfloor n/6 \rfloor^2 + \lfloor n/6 \rfloor}{2} \end{aligned}$$

For the small case $n = 14$, direct addition and the formula both yield $S_{A\cup B} = 68$.

Venn Diagrams for 3 or More Subsets

Venn diagrams are quite commonly drawn for three overlapping subsets, and they have this general definition.

DEF: A family of n simple closed curves (typically circles or ellipses) in the plane, whose interior regions represent some subsets $A_1, A_2, \ldots, A_n$ of a set A within a domain U, is called a ***Venn diagram***, after the logician John Venn (1834-1923).

TERMINOLOGY: The domain U from which both the subsets A and B are drawn is commonly called the *universal set*.

Example 3.6.3: Eurasian Translators, Inc., employs 15 expert linguists fluent in at least two of the three languages Armenian, Bulgarian, and Czech. Of these,

$$\begin{aligned} S_{A\cap B} &= 5 \quad \text{speak Armenian and Bulgarian} \\ S_{A\cap C} &= 7 \quad \text{speak Armenian and Czech} \\ \text{and} \quad S_{B\cap C} &= 9 \quad \text{speak Bulgarian and Czech} \end{aligned}$$

How many speak all three languages? Figure 3.6.2 is the relevant Venn diagram.

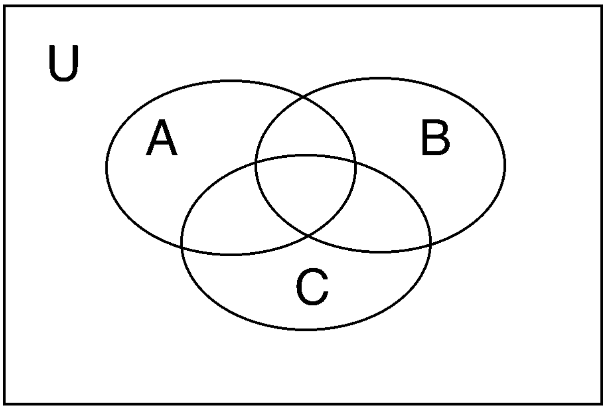

Fig 3.6.2 Venn diagram for three overlapping subsets.

Whereas 15 is the given number of linguists fluent in two or more of the three languages, the sum

$$S_{A\cap B} + S_{A\cap C} + S_{B\cap C} \;=\; 5+7+9 \;=\; 21$$

of the numbers corresponding to the three intersection-regions for which data are given triple-counts the contribution $S_{A\cap B\cap C}$ in the triple intersection at the center of the diagram and counts all the other translators only once.

Thus, subtracting 15, thereby excluding the total number of translators who speak at least two of the languages by the calculation

$$2\,S_{A\cap B\cap C} \;=\; 21 - 15 \;=\; 6$$

yields the result

$$2\,S_{A\cap B\cap C} \;=\; 6$$

from which one concludes that

$$S_{A\cap B\cap C} = 3$$

It is helpful to check such a result by inserting numbers into the regions of the Venn diagram. In this case, the number 3 is inserted into the centermost region, representing the population of the region $A \cap B \cap C$ in Figure 3.6.3. Then it must be excluded from the populations given for composite regions $A \cap B$, $A \cap C$, and $B \cap C$, in order to obtain populations for the simple regions they contain.

NOTATION: The complement of a set X in a domain U is denoted $\overline{X}$.

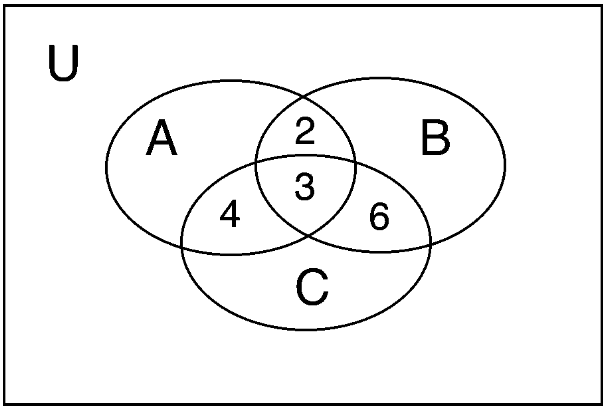

Fig 3.6.3 Inserting numbers into regions of a Venn diagram.

We observe that all of the inserted numbers are consistent with the original data as well as with the derived population of $A \cap B \cap C$.

$$\begin{array}{rrcccccl} & S_{A\cap B} & = & 5 & = & 2+3 & = & S_{A\cap B\cap\overline{C}} + S_{A\cap B\cap C} \\ & S_{A\cap C} & = & 7 & = & 4+3 & = & S_{A\cap\overline{B}\cap C} + S_{A\cap B\cap C} \\ \text{and} & S_{B\cap C} & = & 9 & = & 6+3 & = & S_{\overline{A}\cap B\cap C} + S_{A\cap B\cap C} \end{array}$$

Context for Inclusion-Exclusion

A more general context of *inclusion-exclusion* evaluations is a domain U, a real-valued function $f : U \to \mathbb{R}$, and a representation

$$A \;=\; \bigcup_{k=1}^{n} A_k$$

of set A as a union of subsets A_k, regarded like a Venn diagram with n mutually intersecting subsets. (Some of the regions may be empty.)

Remark: Quite often, the function $f : U \to \mathbb{R}$ is the constant function $f(x) = 1$, in which case the evaluation amounts to calculating the cardinality of a region.

NOTATION: The intersection of two sets A_i and A_j may be denoted by the juxtaposition $A_i A_j$.

DEF: An intersection $A_{i_1} A_{i_2} \cdots A_{i_r}$ is called an ***r-fold intersection*** of the family $\{A_k\}$.

Formulas for Inclusion-Exclusion

As illustrated by Example 3.6.3, evaluating sums over combinations of regions in Venn diagrams takes some care. Fortunately, such evaluations can usually be reduced to the application of two or three general inclusion-exclusion equations for sums over single regions.

Thm 3.6.1 [Exclude-All Equation for Set Size]. *Let* $A_1, \ldots, A_n$ *be subsets of a set* U*, with*

$$A = \bigcup_{k=1}^{n} A_k \quad \text{and} \quad S_r = \sum_{i_1,\ldots,i_r \in [1:n]} |A_{i_1} \cdots A_{i_r}|$$

so that, for $r = 1, \ldots, n$*, the number* S_r *is the sum of the cardinalities of all* r*-fold intersections of the family* $\{A_k\}$*. Then*

$$|\overline{A}| = \left|\overline{A_1}\,\overline{A_2} \cdots \overline{A_n}\right| = |U| + \sum_{k=1}^{n} (-1)^k S_k$$

Proof: First suppose that the element $x \in U$ lies in none of the sets A_j. Then x is counted once on the left side of the equation, and it is counted in the formula on the right side only by the summand $|U|$, and not by any summand S_k.

Now suppose that x lies in exactly m of the subsets A_j, with $m > 0$. Accordingly x is not counted on the left side of the equation. On the right side, it is counted $\binom{m}{k}$ times by S_k, since there are $\binom{m}{k}$ ways to choose k sets from the m sets A_j that contain x, and x is also counted once by $|U|$. Thus, its net count on the right side is

$$\begin{aligned} 1 + \sum_{k=1}^{m} (-1)^k \binom{m}{k} &= \sum_{k=0}^{m} (-1)^k \binom{m}{k} \\ &= (1-z)^m \Big|_{z=1} = 0 \qquad \diamondsuit \end{aligned}$$

The other main incl-excl formula is derivable by the same approach, or, as shown here, as a corollary of Thm 3.6.1.

Cor 3.6.2 [Include-All Equation for Set Size]. *Let $A_1, \ldots, A_n$ be subsets of a set U, with*

$$A = \bigcup_{k=1}^{n} A_k \quad \text{and} \quad S_r = \sum_{i_1,\ldots,i_r \in [1:n]} |A_{i_1} \cdots A_{i_r}|$$

so that, for $r = 1, \ldots, n$, the number S_r is the sum of the cardinalities of all r-fold intersections of the family $\{A_k\}$. Then

$$|A| = \sum_{k=1}^{n} (-1)^{k-1} S_k$$

Proof: Observe that the universal set U is the disjoint union of the set A and the set $\overline{A_1}\,\overline{A_2} \cdots \overline{A_n}$. Therefore,

$$|U| = |A| + \left|\overline{A_1}\,\overline{A_2} \cdots \overline{A_n}\right|$$

and, accordingly,

$$|A| = |U| - \left|\,\overline{A_1}\,\overline{A_2}\,\cdots\,\overline{A_n}\,\right|$$

and then, by Theorem 3.6.1,

$$= \left(\left|\,\overline{A_1}\,\overline{A_2}\,\cdots\,\overline{A_n}\,\right| - \sum_{k=1}^{n}(-1)^k S_k\right) - \left|\,\overline{A_1}\,\overline{A_2}\,\cdots\,\overline{A_n}\,\right|$$

$$= \sum_{k=1}^{n}(-1)^{k-1} S_k \qquad \diamondsuit$$

Thm 3.6.3 provides an inclusion-exclusion formula for the sum of the values of an arbitrary function $f : U \to \mathbb{R}$ on the domain U, not simply for counting the size of a set.

Thm 3.6.3 [General Exclude-All Eq]. *Let $A_1, \ldots, A_n$ be subsets of a set U, with*

$$A = \bigcup_{k=1}^{n} A_k$$

and let $f : U \to \mathbb{R}$ be a real-valued function. Let the sum

$$S_r = \sum_{i_1,\ldots,i_r \in [1:n]} \; \sum_{x \in A_{i_1} \cdots A_{i_r}} f(x)$$

be taken over all r-fold intersections of the family $\{A_k\}$. Then

$$\sum_{x \in \overline{A_1} \cdots \overline{A_n}} f(x) = \sum_{x \in U} f(x) + \sum_{k=1}^{n}(-1)^k S_k$$

Proof: The proof is a straightforward modification of the proof of the Exclude-All Equation for set sizes. ♢

In the remainder of this section, the two main inclusion-exclusion formulas are applied to various combinatorial problems.

Stirling Subset Numbers

Although there are various similarities between Stirling numbers and binomial coefficients, there is no known closed formula for Stirling numbers of either kind, unlike the situation for binomial coefficients. However, there is a summation formula for a Stirling subset number, whose derivation by inclusion-exclusion is our immediate objective. The ideas involved are encapsulated in the following example.

Example 3.6.4: The Stirling subset number $\left\{ {5 \atop 4} \right\}$ is the number of ways to distribute a set of 5 objects into 4 cells with no cell left empty. For a problem this small, listing cases is easy enough, but it is instructive to apply inclusion-exclusion. Toward that objective, for $i = 1, 2, 3, 4$, let A_i be the set of distributions with box i left empty. Clearly,

$$\begin{aligned} |A_i| &= 3^5 && \text{for } i = 1, 2, 3, 4 \\ |A_i A_j| &= 2^5 && \text{for } i \neq j \\ |A_i A_j A_k| &= 1^5 && \text{for mutually distinct } i, j, k \end{aligned}$$

Moreover,

$$S_k = \binom{4}{k}(4-k)^5 \tag{3.6.1}$$

since there are $\binom{4}{k}$ ways to choose k of the subsets A_i from the collection of four such subsets, and each intersection $A_{i_1} A_{i_2} \cdots A_{i_k}$ contains $(4-k)^5$ objects. Furthermore,

$$|\overline{A_1}\,\overline{A_2}\,\overline{A_3}\,\overline{A_4}| = \left\{ {5 \atop 4} \right\} 4! \tag{3.6.2}$$

since each distribution with none of the boxes left empty amounts to assigning the labels $1, 2, 3, 4$ to the cells of a partition. Finally, if U is the set of all ways to distribute 5 objects into 4 cells, we have

$$|U| = 4^5 \tag{3.6.3}$$

When we substitute into the Exclude-All Equation

$$|\overline{A_1}\,\overline{A_2}\,\overline{A_3}\,\overline{A_4}| = |U| - S_1 + S_2 - S_3 + S_4$$

the values from Equations (3.6.1), (3.6.2), and (3.6.3), we obtain the equation

$$\begin{aligned} \left\{ {5 \atop 4} \right\} 4! &= 4^5 - \binom{4}{1}3^5 + \binom{4}{2}2^5 - \binom{4}{3}1^5 + \binom{4}{4}0^5 \\ &= 1024 - 972 + 192 - 4 = 240 \\ \Rightarrow \quad \left\{ {5 \atop 4} \right\} &= \frac{240}{4!} = 10 \end{aligned}$$

A confirming observation is that, since two of the elements are paired, and since the others have cells to themselves, clearly

$$\left\{ {5 \atop 4} \right\} = \binom{5}{2} = 10$$

In a similar manner, an inclusion-exclusion analysis leads to an identity for the Stirling subset numbers

$$\left\{ {n \atop m} \right\}$$

Proof of the following theorem simply generalizes the steps and calculations that we have just completed.

Theorem 3.6.4. *Let n and k be a pair of non-negative integers. Then*

$$\left\{ {n \atop k} \right\} k! = \sum_{j=0}^{k} (-1)^j \binom{k}{j} (k-j)^n$$

Proof: For $i = 1, 2, \ldots, k$, let A_i be the set of distributions of n distinct objects into k *distinct* boxes with box i left empty. Clearly,

$$|A_i| = (k-1)^n \qquad \text{for } i = 1, 2, \ldots, k$$

and, more generally, for any $j \in [1, k]$

$$|A_{i_1} A_{i_2} \cdots A_{i_j}| = (k-j)^n \qquad \text{for mutually distinct } i_1, i_2, \ldots, i_j$$

Since there are $\binom{k}{j}$ ways to choose the mutually distinct $i_1, i_2, \ldots, i_j$, and since S_j is the sum of the numbers of ways to leave j specific boxes empty (with others possibly empty also), it follows, by analogy to Eq. (3.6.1), that

$$S_j = \binom{k}{j}(k-j)^n \qquad (3.6.1')$$

Furthermore,

$$|\overline{A_1}\,\overline{A_2} \cdots \overline{A_k}| = \left\{ {n \atop k} \right\} k! \qquad (3.6.2')$$

since each distribution with none of the k boxes left empty amounts to assigning the labels $1, 2, \ldots, k$ to the cells of a partition. Finally, if U is the set of all ways to distribute n objects into k cells, we have

$$|U| = k^n = \binom{k}{0}(k-0)^n \qquad (3.6.3')$$

Substituting the values from Equations (3.6.1′), (3.6.2′), and (3.6.3′) just above into the Exclude-All Equation

$$|\overline{A_1}\,\overline{A_2} \cdots \overline{A_k}| = |U| - S_1 + S_2 + \cdots + (-1)^k S_k$$

we obtain the identity

$$\left\{ {n \atop k} \right\} k! = \sum_{j=0}^{k} (-1)^j \binom{k}{j}(k-j)^n \qquad \diamondsuit$$

Derangements

Inclusion-exclusion is also helpful in analyzing the derangement recurrence.

REVIEW FROM §2.1:

- A ***derangement*** is a permutation π with no fixed points.
- The ***derangement number*** D_n is the number of derangements of the integer interval $[1 : n]$.
- The ***derangement recurrence*** (see also §5.4) is

$$D_0 = 1, \quad D_1 = 0; \tag{3.6.4a}$$
$$D_n = (n-1)D_{n-1} + (n-1)D_{n-2} \tag{3.6.4b}$$

Example 3.6.5: In the classical ***hatcheck problem***, each of n persons leaves a hat in the cloakroom, but the hatchecks are lost, and the n hats are redistributed randomly. It asks, what is the probability that no hat goes to its rightful owner? This problem is recognizable as a homespun version of calculating the proportion of permutations of n objects that are derangements.

If U is the set of all possible hat distributions, then

$$|U| = n! \tag{3.6.5}$$

To calculate the number D_n of derangements, let A_i be the set of permutations in which hat i goes to its rightful owner. Then

$$D_n = |\overline{A_1}\,\overline{A_2} \cdots \overline{A_n}| \qquad (3.6.6)$$

and

$$|A_i| = (n-1)!$$

More generally,

$$|A_{i_1} A_{i_2} \cdots A_{i_r}| = (n-r)!$$

which implies that

$$S_k = \binom{n}{k}(n-k)! \qquad (3.6.7)$$

When the Exclude-All Equation

$$|\overline{A_1}\,\overline{A_2} \cdots \overline{A_n}| = |U| + \sum_{k=1}^{n}(-1)^k S_k$$

is combined with Equations (3.6.5), (3.6.6), and (3.6.7), we obtain

$$\begin{aligned} D_n &= n! + \sum_{k=1}^{n}(-1)^k \binom{n}{k}(n-k)! \\ &= \sum_{k=0}^{n}(-1)^k \frac{n!}{k!} \qquad (3.6.8) \end{aligned}$$

Substituting $n = 0$ and $n = 1$ into Eq. (3.6.8), we obtain

$$D_0 = \sum_{k=0}^{0}(-1)^0 \frac{0!}{k!}$$

$$= (-1)^0 \frac{0!}{0!} = 1$$

and

$$\begin{aligned} D_1 &= \sum_{k=0}^{1} (-1)^k \frac{1!}{k!} \\ &= (-1)^0 \frac{1!}{0!} + (-1)^1 \frac{1!}{0!} = 1 + (-1) = 0 \end{aligned}$$

which establishes that equation (3.6.8) satisfies the initial conditions (3.6.4a) of the derangement recurrence. Moreover, assuming that equation (3.6.8) satisfies the recurrence for D_{n-1} and D_{n-2}, we confirm by the following calculation that it also satisfies the recurrence for D_n.

$$\begin{aligned} &(n-1)D_{n-1} + (n-1)D_{n-2} \\ &\quad= (n-1)\sum_{k=0}^{n-1}(-1)^k \frac{(n-1)!}{k!} + (n-1)\sum_{k=0}^{n-2}(-1)^k \frac{(n-2)!}{k!} \\ &\quad= \sum_{k=0}^{n-1}(-1)^k \frac{n!}{k!} - \sum_{k=0}^{n-1}(-1)^k \frac{(n-1)!}{k!} + \sum_{k=0}^{n-2}(-1)^k \frac{(n-1)!}{k!} \\ &\quad= \sum_{k=0}^{n-1}(-1)^k \frac{n!}{k!} - (-1)^{n-1} \frac{(n-1)!}{(n-1)!} \\ &\quad= \sum_{k=0}^{n-1}(-1)^k \frac{n!}{k!} + (-1)^n \frac{n!}{n!} \\ &\quad= \sum_{k=0}^{n}(-1)^k \frac{n!}{k!} \end{aligned}$$

Remark: We observe that

$$D_n = \sum_{k=0}^{n} (-1)^k \frac{n!}{k!} \tag{3.6.8}$$

implies that

$$\frac{D_n}{n!} = \sum_{k=0}^{n} (-1)^k \frac{1}{k!} \underset{n\to\infty}{\longrightarrow} e^{-1}$$

Thus, one might approximate the value of e^{-1}, and hence, of the number e, by generating random permutations and counting the proportion that are derangements.

Counting Bipartite Matchings

In the rest of this section, a prior acquaintance with graph theory would be helpful.

REVIEW FROM §0.6:

- A ***bipartite graph*** G is a graph whose vertex set can be partitioned into two subsets X and Y s.t. every edge has one vertex in X and the other in Y.

PREVIEW OF §8.6:

- A ***matching*** in a graph is a set of edges such that no two edges have an endpoint in common.
- A ***perfect matching*** in a graph is a matching in which every vertex is the endpoint of one of the edges.

Example 3.6.6: In the bipartite graph G of Fig 3.6.4, there are five perfect matchings:

one with $f(1) = a$ (shown with thicker edges);

three with $f(1) = b$;

and one with $f(1) = c$.

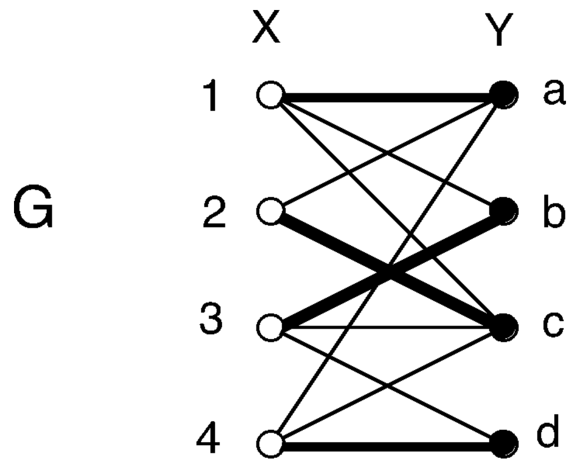

Fig 3.6.4 Perfect matching in a bipartite graph.

Let U be the total set of bijections $X \to Y$. Then

$$|U| = 4! = 24 \tag{3.6.9}$$

A bijection $X \to Y$ is *consistent* with the bipartite graph G if it is representable as a perfect matching in G. For $i = 1, 2, 3, 4$, let A_i be the number of bijections $f : X \to Y$ such that the assignment $i \mapsto f(i)$ is inconsistent with the graph G, that is, such that vertex $f(i)$ is not adjacent to vertex i.

For each choice of a vertex of Y that is not adjacent to vertex i, there are $3!$ bijections $X \to Y$, corresponding to the 3! ways to assign the other 3 vertices of X to the remaining 3 vertices of Y. Thus,

$$|A_i| = (4 - deg(i)) \cdot 3!$$

and there are similar formulas for multiple inconsistencies.

$$|A_1| = |A_3| = |A_4| = 1 \cdot 3! \text{ and } |A_2| = 2 \cdot 3!$$

$$|A_1A_2| = |A_1A_3| = |A_1A_4| = |A_2A_4| = |A_3A_4| = 2!$$

$$\text{and } |A_2A_3| = 2 \cdot 2!$$

$$|A_1A_2A_3| = |A_1A_3A_4| = |A_2A_3A_4| = 1 \text{ and } |A_1A_2A_4| = 0$$

$$\Rightarrow \quad S_1 = 30,\ S_2 = 14,\ S_3 = 3,\ S_4 = 0 \quad (3.6.10)$$

Therefore, by using (3.6.9) and (3.6.10) with the Exclude-All Equation, the number of perfect matchings is shown to be

$$\begin{aligned} |\overline{A_1}\,\overline{A_2}\,\overline{A_3}\,\overline{A_4}| &= |U| - S_1 + S_2 - S_3 + S_4 \\ &= 24 - 30 + 14 - 3 + 0 \\ &= 5 \end{aligned}$$

which agrees with our ad hoc count at the outset.

An alternative representation of this counting problem is the chessboard of Figure 3.6.5. Observe that a square is shaded if and only if it is forbidden to match the vertex corresponding to its row to the vertex corresponding to its column. Each perfect matching corresponds to a selection of one unshaded square in each row, such that there is at most one selection in each column.

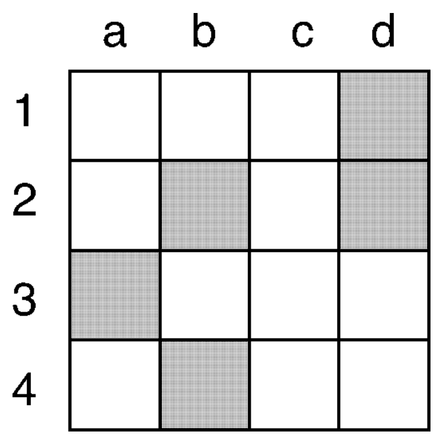

Fig 3.6.5 Chessboard representation of a bipartite matching problem.

Remark: The method given here is applicable also to counting complete matchings of a bipartite graph when one part has more vertices than the other.

Chromatic Polynomials

An algebraic invariant called the *chromatic polynomial* of a graph can be calculated by inclusion-exclusion.

PREVIEW OF §8.3:

- A ***vertex-coloring of a graph*** G in the set $[1:n]$, often simply called a ***coloring***, is a function $f : V_G \to [1:n]$.
- A ***proper vertex-coloring of a graph*** is a coloring such that no two adjacent vertices have the same color.

DEF: The ***chromatic polynomial*** $P(G,t)$ of a graph G is the function whose value at the integer t is the number of proper colorings of G with at most t colors.

As a preliminary to a more systematic approach, we consider an *ad hoc* construction of a chromatic polynomial. It illustrates why the function $P(G,n)$ is a polynomial.

Example 3.6.7: The graph $K_{1,2}$ requires at least two colors for a proper coloring. We observe that, given two colors, exactly two proper 2-colorings are possible, one of which is illustrated in Figure 3.6.6. We write $p_2 = 2$. Given three colors, exactly six 2-colorings (i.e., 3!) are possible, so we write $p_3 = 6$.

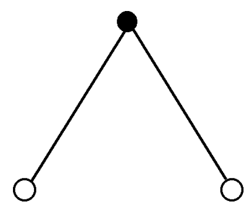

Fig 3.6.6 A proper 2-coloring for the bipartite graph $K_{1,2}$.

For any positive integer t, the # ways to choose two colors is $\binom{t}{2}$ and the number of ways to choose three colors is $\binom{t}{3}$, By Rule of Product and Rule of Sum, it follows that the number of proper colorings with t colors is

$$\begin{aligned} p_2\binom{t}{2} + p_3\binom{t}{3} &= 2\cdot\frac{t(t-1)}{2!} + 6\cdot\frac{t(t-1)(t-2)}{3!} \\ &= \left(t^2-t\right) + \left(t^3-3t^2+2t\right) \\ &= t^3 - 2t^2 + t \qquad (3.6.11) \end{aligned}$$

In general, it may be computationally difficult to determine the exact numbers of proper colorings

$$p_1 \quad p_2 \quad \cdots \quad p_n$$

for an n-vertex graph G, or even to decide the *chromatic number*, i.e., the smallest positive value. However, whatever those numbers may be, the chromatic polynomial is

$$P(G,t) \;=\; p_1\binom{t}{2} + p_2\binom{t}{2} + \cdots + p_n\binom{t}{n}$$

Example 3.6.7, cont.: To recalculate the chromatic polynomial of the graph $K_{1,2}$ by inclusion-exclusion, its two edges are labeled 1 and 2, as shown in Figure 3.6.7.

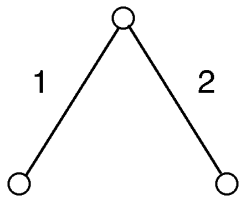

Fig 3.6.7 An edge-labeling for the bipartite graph $K_{1,2}$.

Let U be the set of all colorings of $K_{1,2}$ with at most t colors. Let A_1 be the set of such colorings in which the endpoints of edge 1 have the same color, and let A_2 be the set of such colorings in which the endpoints of edge 2 have the same color. Then

$$P(K_{1,2},t) \;=\; |U| - |A_1\,A_2|$$

This is a job for the Exclude-All Equation. Evidently, $|U| = t^3$.

To calculate $|A_1|$, we recognize that there are t possible choices of a color for both endpoints of edge 1, and then another t possible choices for the color of the remaining vertex. Clearly, this holds also for $|A_2|$. Thus,

$$\begin{aligned} |A_1| &= |A_2| = t^2 \\ \text{and} \quad S_1 &= |A_1| + |A_2| = 2t^2 \end{aligned}$$

Any coloring in $A_1 \cap A_2$ has the same color at both endpoints of edge 1 and the same color at both ends of edge 2. Since these two edges share an endpoint, all three vertices of $K_{1,2}$ must have the same color. There are t possible choices for this color. Thus,

$$\begin{aligned} |A_1\, A_2| &= t \\ \text{and} \quad S_2 = |A_1\, A_2| &= t \end{aligned}$$

We now complete the recalculation,

$$\begin{aligned} |\,\overline{A_1}\;\overline{A_2}\,| &= |U| - S_1 + S_2 \\ &= t^3 - 2t^2 + t \end{aligned} \qquad (3.6.12)$$

which agrees with (3.6.11).

Example 3.6.8: To calculate the chromatic polynomial $P(K_4, t)$ of the complete graph K_4 by inclusion-exclusion, label its its six edges with numbers $1, \ldots, 6$, as shown in Figure 3.6.8.

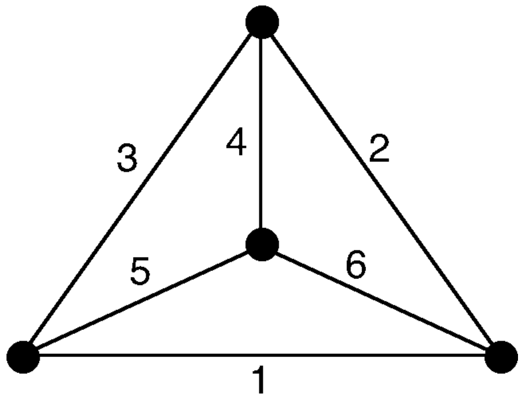

Fig 3.6.8 An edge-labeling of the complete graph K_4.

Let U be the set of all colorings of K_4 with colors in $[1:t]$. Then

$$|U| = t^4$$

Next, let A_i be the set of colorings in $[1:t]$ such that the endpoints of edge i have the same color. Then $|A_i| = t^3$, since there are t possibilities for the color of the endpoints of edge i and t possibilities for each of the other two vertices. Since there are 6 edges, it follows that

$$S_1 = |A_1| + |A_2| + \cdots + |A_6| = 6t^3$$

There are $\binom{6}{2} = 15$ ways to choose a pair of edges, i and j. For 3 of these pairs, edges i and j have no vertex in common, in which case a coloring in A_iA_j may use t colors for the endpoints of edge i and t colors for the endpoints of edge j, yielding t^2 possibilities. For the 12 pairs of edges that have a vertex in common, there are t choices for the color of the three vertices in the union of their endpoint sets and t choices for the remaining vertex, again yielding t^2 possibilities. Thus,

$$S_2 = 15t^2$$

There are $\binom{6}{3} = 20$ ways to choose three edges. Exactly 4 of these 20 triples form a 3-cycle. There are t choices for the color of all three vertices in that 3-cycle and t choices for the remaining vertex. The other 16 edge-triples form a connected subgraph (a *spanning tree*) that contains all four vertices of K_4, so all four must get the same color, for which there are t choices. Accordingly,

$$S_3 = 4t^2 + 16t$$

A subset of four or more edges must contain all the vertices of K_4. It follows that

$$S_4 = \binom{6}{4}t = 15t$$

$$S_5 = \binom{6}{5}t = 6t$$

$$\text{and} \quad S_6 = \binom{6}{6}t = t$$

By the Exclude-All Formula,

$$\begin{aligned} P(K_4, t) &= |U| - S_1 + S_2 - S_3 + S_4 - S_5 + S_6 \\ &= t^4 - 6t^3 + 15t^2 - (4t^2 + 16t) + 15t - 6t + t \\ &= t^4 - 6t^3 + 11t^2 - 6t \end{aligned}$$

Remark: There are circumstances where the Exclude-All Formula is an excellent way to calculate chromatic polynomials, which are not revealed by these small examples. For instance, it can be used to prove that the chromatic polynomial of any n-vertex tree is $t(t-1)^{n-1}$.