ANALYTIC COMBINATORICS BASIC COMPLEX ASYMPTOTICS

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PREFACE

Analytic Combinatorics aims at predicting precisely the asymptotic properties of structured combinatorial configurations, through an approach that bases itself extensively on analytic methods. Generating functions are the central objects of the theory.

Analytic combinatorics starts from an exact enumerative description of combinatorial structures by means of generating functions, which make their first appearance as purely formal algebraic objects. Next, generating functions are interpreted as analytic objects, that is, as mappings of the complex plane into itself. In this context, singularities play a key rôle in extracting a function's coefficients in asymptotic form and extremely precise estimates result for counting sequences. This chain is applicable to a large number of problems of discrete mathematics relative to words, trees, permutations, graphs, and so on. A suitable adaptation of the theory finally opens the way to the analysis of parameters of large random structures.

Analytic combinatorics can accordingly be organized based on three components:

- Symbolic Methods develops systematic "symbolic" relations between some of the major constructions of discrete mathematics and operations on generating functions which exactly encode counting sequences.
- Complex Asymptotics elaborates a collection of methods by which one can extract asymptotic counting informations from generating functions, once these are viewed as analytic transformations of the complex domain (as "analytic" also known as "holomorphic" functions). Singularities then appear to be a key determinant of asymptotic behaviour.
- Random Structuress concerns itself with probabilistic properties of large random structures—which properties hold with "high" probability, which laws govern randomness in large objects? In the context of analytic combinatorics, this corresponds to a deformation (adding auxiliary variables) and a perturbation (examining the effect of small variations of such auxiliary variables) of the standard enumerative theory.

The approach to quantitative problems of discrete mathematics provided by analytic combinatorics can be viewed as an *operational calculus* for combinatorics. The booklets, of which this is the second installment, expose this view by means of a very large number of examples concerning classical combinatorial structures (like words, trees, permutations, and graphs). What is aimed at eventually is an effective way of quantifying "metric" properties of large random structures. Accordingly, the theory is susceptible to many applications, within combinatorics itself, but, perhaps more importantly, within other areas of science where discrete probabilistic models recurrently surface, like statistical physics, computational biology, or electrical engineering. Last but not least, the analysis of algorithms and data structures in computer science has served and still serves as an important motivation in the development of the theory.

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The present booklet specifically exposes *Singular Combinatorics*, which is a unified analytic theory dedicated to the process of extractic asymptotic information from counting generating functions. As it turns out, a collection of general (and simple) theorems provide a systematic translation mechanism between generating functions and asymptotic forms of coefficients. Two chapters compose this booklet. Chapter IV serves as an *introduction to complex-analytic methods* and proceeds with the treatment of *meromorphic functions*, that is, functions whose only singularities are poles, *rational functions* being the simplest case. Chapter V develops *applications of rational and meromorphic asymptotics*, with numerous applications related to words and languages, walks and graphs, as well as permutations. [Future chapters will treat Singularity Analysis (Chapter VI) and its Applications (Chapter VII).]

CHAPTER IV

Complex Analysis, Rational and Meromorphic Asymptotics

The shortest path between two truths in the real domain passes through the complex domain.

— JACQUES HADAMARD¹

Generating functions are a central concept of combinatorial theory. So far, they have been treated as formal objects, that is, as formal power series. The major theme of Chapters I–III has indeed been to demonstrate how the algebraic structure of generating functions directly reflects the structure of combinatorial classes. From now on, we examine generating functions in the light of *analysis*. This means assigning *values* to the variables that appear in generating functions.

Comparatively little benefit results from assigning only real values to the variable z that figures in a univariate generating function. In contrast assigning *complex* values turns out to have serendipitous consequences. In so doing, a generating function becomes a geometric transformation of the complex plane. This transformation is very regular near the origin—one says that it is analytic or holomorphic. In other words, it only effects initially a smooth distortion of the complex plane.

Farther away from the origin, some "cracks" start appearing in the picture. These cracks—the dignified name is "singularities"—correspond to the disapperance of smoothness. What happens is that knowledge of a function's singularities provide a wealth of information regarding the function's coefficients, and especially their asymptotic rate of growth. Adopting a geometric point of view has a large pay-off.

By focussing on singularities, analytic combinatorics treads in the steps of many respectable older areas of mathematics. For instance, Euler recognized that the fact for the Riemann zeta function $\zeta(s)$ to become infinite at 1 implies the existence of infinitely many prime numbers, while Riemann, Hadamard, and de la Vallée-Poussin uncovered much deeper connections between quantitative properties of the primes and singularities of $1/\zeta(s)$.

In this chapter, we start by recalling the elementary theory of analytic functions and their singularities in a style tuned to the needs of combinatorial theory. Cauchy's integral formula expresses coefficients of analytic functions as contour integrals. Suitable uses of Cauchy's integral formula then make it possible to estimate such coefficients by suitably selecting the contour of integration. For the fairly common case of functions that have singularities at a finite distance, the *exponential growth* formula relates the *location* of the singularities closest to the origin (these are also known as "dominant" singularities then dictates the network of the singularities.

¹Quoted in The Mathematical Intelligencer, v. 13, no. 1, Winter 1991.

the fine structure of the asymptotic of the function's coefficients, especially the *subexponential factors* involved. In this chapter we carry out this programme for rational functions and meromorphic functions, where the latter are defined by the fact their singularities are of the polar type.

Elementary techniques permit us to estimate asymptotically counting sequences, when these are already presented to us in closed form or as simple combinatorial sums. The methods to be exposed require no such explicit forms of counting coefficients to be available. They apply to almost any conceivable combinatorial generating function that has a decent mathematical expression—we already know from Chapters I–III that this covers a very large fragment of elementary combinatorics. In a large number of cases, complexanalytic methods can even be applied to generating functions only accessible *implicitly* from *functional equations*. This paradigm will be extensively explored in this chapter with applications found in denumerants, derangements, surjections, alignments, and several other structures introduced in Chapters I–III.

IV.1. Generating functions as analytic objects

Generating functions, considered previously as purely *formal* objects subject to algebraic operations, are now going to be interpreted as *analytic* objects. In so doing one gains an easy access to the asymptotic form of their coefficients. This informal section offer a glimpse of themes that form the basis of this chapter and the next one.

In order to introduce the subject softly, let us start with two simple generating functions, one, f(z), being the OGF of the Catalan numbers (starting at index 1), the other, g(z), being the EGF of derangements:

(1)
$$f(z) = \frac{1}{2} \left(1 - \sqrt{1 - 4z} \right), \qquad g(z) = \frac{\exp(-z)}{1 - z}$$

At this stage, the forms above are merely compact descriptions of formal power series built from the elementary series

$$(1-u)^{-1} = 1+u+u^2+\cdots, \qquad (1-u)^{1/2} = 1-\frac{1}{2}u-\frac{1}{8}u^2-\cdots,$$

$$\exp(u) = 1+\frac{1}{1!}u+\frac{1}{2!}u^2+\cdots,$$

by standard composition rules. Accordingly, the coefficients of both GFs are known in explicit form

$$f_n := [z^n]f(z) = \frac{1}{n} \binom{2n-2}{n-1}, \qquad g_n := [z^n]g(z) = \left(\frac{1}{0!} - \frac{1}{1!} + \frac{1}{2!} - \dots + \frac{(-1)^n}{n!}\right).$$

Next, Stirling's formula and comparison with the alternating series giving exp(-1) provide respectively

(2)
$$f_n \underset{n \to \infty}{\sim} \frac{4^n}{\sqrt{\pi n^3}}, \qquad g_n = \underset{n \to \infty}{\sim} e^{-1} \doteq 0.36787.$$

Our purpose is to examine, heuristically for the moment, the relationship between the asymptotic forms (2) and the structure of the corresponding generating functions in (1).

Granted the growth estimates available for f_n and g_n , it is legitimate to substitute in the power series expansions of the GFs f(z) and g(z) any real or complex value of a small enough modulus, the upper bounds on modulus being $\rho_f = \frac{1}{4}$ (for f) and $\rho_g = 1$ (for g). Figure 1 represents the graph of the resulting functions when such real values are assigned to z. The graphs are smooth, representing functions that are differentiable any



FIGURE 1. Left: the graph of the Catalan OGF, f(z), for $z \in (-\frac{1}{4}, +\frac{1}{4})$; right: the graph of the derangement EGF, g(z), for $z \in (-1, +1)$.

number of times for z interior to the interval $(-\rho, +\rho)$. However, at the right boundary point, smoothness stops: g(z) become infinite at z = 1, and so it even ceases to be finitely defined; f(z) does tend to the limit $\frac{1}{2}$ as $z \to (\frac{1}{4})^-$, but its derivative becomes infinite there. Such special points at which smoothness stops are called *singularities*, a term that will acquire a precise meaning in the next sections.

Observe also that, by the usual process of analysis, f(z) and g(z) can be *continued* in certain regions, when use is made of the global expressions (1) while exp and $\sqrt{}$ are assigned their usual real-analytic interpretation; for instance:

$$f(-1) = \frac{1}{2} \left(1 - \sqrt{5} \right), \qquad g(-2) = \frac{e^2}{3}.$$

Such "continuation" properties (to the complex realm) will prove essential in developing efficient methods for coefficient asymptotics.

One may proceed similarly with complex numbers, starting with numbers whose modulus is less than the radius of convergence of the series defining the GF. Figure 2 displays the images of regular grids by f and g. This illustrates the fact that a regular grid transforms into an orthogonal network of curves and more precisely that f and g preserve angles this property corresponds to complex differentiability and is equivalent to analyticity to be introduced shortly. The singularity of f is clearly perceptible on the right of its diagram, since, at $z = \frac{1}{4}$ corresponding to $f(z) = \frac{1}{2}$, the function f folds lines and divides angles by a factor of 2.

Let us now turn to coefficient asymptotics. As is expressed by (2), the coefficients f_n and g_n each belong to a general asymptotic type,

$$A^n\theta(n),$$

corresponding to an exponential growth factor A^n modulated by a tame factor $\theta(n)$, which is subexponential; compare with (2). Here, one has A = 4 for f_n and A = 1 for g_n ; also, $\theta(n) = \frac{1}{4}(\sqrt{\pi n^3})^{-1}$ for f_n and $\theta(n) = e^{-1}$ for g_n . Clearly, A should be related to the radius of convergence of the series. We shall see that, on very general grounds, the exponential rate of growth is given by $A = 1/\rho$, where ρ is the first singularity encountered along the positive real axis. In addition, under general complex-analytic conditions, it will be established that $\theta(n) = O(1)$ is systematically associated to a simple pole of the generating function, while $\theta(n) = O(n^{-3/2})$ systematically arises from a singularity that



FIGURE 2. The images of regular grids by f(z) (left) and g(z) (right).

is of the square-root type. In summary, as this chapter and the next ones will copiously illustrate, one has:

Fundamental principle of complex coefficient asymptotics. The location of a function's singularities dictates the exponential growth of the function's coefficient, A^n , while the nature of the function at its singularities determines the subexponential factor, $\theta(n)$.

Observe that the rescaling rule,

$$[z^n]f(z) = \rho^{-n}[z^n]f(\rho z),$$

enables one to normalize functions so that they are singular at 1, and so "explains" the fact that the location of a function's singularities should influence the coefficients' approximation by exponential factors. Then various theorems, starting with Theorems IV.6 and IV.7, provide sufficient conditions under which the following central implication is valid,

(3)
$$h(z) \sim \sigma(z) \implies [z^n]h(z) \sim [z^n]\sigma(z),$$

where h(z) is a function singular at 1 whose Taylor coefficients are to be estimated and $\sigma(z)$ is an approximation near a singularity—usually σ is a much simpler function, typically like $(1-z)^{\alpha} \log^{\beta}(1-z)$ whose coefficients are easy to find. Under such conditions, it suffices to estimate a function locally in order to derive its coefficients asymptotically. In other words, the relation (3) provides a mapping between asymptotic scales of functions near singularities and asymptotics scales of coefficients.

 \triangleright **1.** *Elementary transfers.* Elementary series manipulation yield the following general result: Let h(z) be a power series with radius of convergence > 1 and assume that $h(1) \neq 0$; then one has

$$[z^n]\frac{h(z)}{1-z} \sim h(1), \qquad [z^n]h(z)\sqrt{1-z} \sim -\frac{h(1)}{2\sqrt{\pi n^3}}, \qquad [z^n]h(z)\log\frac{1}{1-z} \sim \frac{h(1)}{n}.$$

See Bender's survey [9] for many similar statements.

▷ 2. Asymptotics of generalized derangements. The EGF of permutations without cycles of length 1 and 2 satisfies

$$j(z) = \frac{e^{-z-z^2/2}}{1-z}$$
 with $j(z) \underset{z \to 1}{\sim} \frac{e^{-3/2}}{1-z}$.

Analogy with derangements suggests (Note 1 can justify it) that $[z^n]j(z) \sim e^{-3/2}$. Here is a table of exact values of $[z^n]j(z)$ (with relative error of the approximation by $e^{-3/2}$ in parentheses):

	n = 5	n = 10	n = 20	n = 50
j_n :	0.2	0.22317	0.2231301600	0.2231301601484298289332804707640122
error:	(10^{-1})	$(2\cdot 10^{-4})$	$(3 \cdot 10^{-10})$	(10^{-33})

The quality of the asymptotic approximation is extremely good. (Such a property is invariably attached to polar singularities.) <1

IV.2. Analytic functions and meromorphic functions

Analytic functions are the primary mathematical concept for complex asymptotics. They can be characterized in two essentially equivalent ways (Subsection IV. 2.1): by means of convergent series expansions (à la Cauchy and Weierstraß) and by differentiability properties (à la Riemann). The first aspect is directly related to the use of generating functions for enumeration; the second one allows for a powerful abstract discussion of closure properties that usually requires little computation. *Meromorphic functions* are nothing but quotients of analytic functions.

Integral calculus with analytic or meromorphic functions (developed in Subsection IV. 2.2) assumes a shape radically different from what it is in the real domain: integrals become quintessentially independent of details of the integration contour, the residue theorem being a prime illustration of this fact. Conceptually, this makes it possible to relate properties of a function at a point (e.g., the coefficients of its expansion at 0) to its properties at another far-away point (e.g., its residue at a pole).

The presentation in this section and the next one is an informal review of basic properties of analytic functions tuned to the needs of asymptotic analysis of counting sequences. For a detailed treatment, we refer the reader to one of the many excellent treatises on the subject, like the books by Dieudonné [28], Henrici [66], Hille [67], Knopp [72], Titchmarsh [109], or Whittaker and Watson [114].

IV.2.1. Basics. We shall consider functions defined in certain *regions* of the complex domain \mathbb{C} . By a region is meant an open subset Ω of the complex plane that is connected. Here are some examples:





Classical treatises teach us how to extend to the complex domain the standard functions of real analysis: polynomials are immediately extended as soon as complex addition and multiplication have been defined, while the exponential is definable by means of Euler's formula, and one has for instance

 $z^{2} = (x^{2} - y^{2}) + 2ixy, \qquad e^{z} = e^{x}\cos y + ie^{x}\sin y,$

if z = x + iy. Both functions are consequently defined over the whole complex plane \mathbb{C} .

The square-root and the logarithm are conveniently described in polar coordinates by

(4)
$$\sqrt{z} = \sqrt{\rho}e^{i\theta/2}, \qquad \log z = \log \rho + i\theta,$$

if $z = \rho e^{i\theta}$. One can take the domain of validity of (4) to be the complex plane slit along the axis from 0 to $-\infty$, that is, restrict θ to the open interval $(-\pi, +\pi)$, in which case the definitions above specify what is known as the *principal determination*. There is no way for instance to extend by continuity the definition of \sqrt{z} in any domain containing 0 in its interior since, for a > 0 and $z \to -a$, one has $\sqrt{z} \to i\sqrt{a}$ as $z \to -a$ from above, while $\sqrt{z} \to -i\sqrt{a}$ as $z \to -a$ from below. This situation is depicted here:



The point z = 0 where two determinations "meet" is accordingly known as a *branch point*. First comes the main notion of an analytic function that arises from convergent series

expansions.

DEFINITION IV.1. A function f(z) defined over a region Ω is analytic at a point $z_0 \in \Omega$ if, for z in some open disc centred at z_0 and contained in Ω , it is representable by a convergent power series expansion

(5)
$$f(z) = \sum_{n \ge 0} c_n (z - z_0)^n.$$

A function is analytic in a region Ω iff it is analytic at every point of Ω .

As derives from an elementary property of power series, given a function f that is analytic at a point z_0 , there exists a disc (of possibly infinite radius) with the property that the series representing f(z) is convergent for z inside the disc and divergent for zoutside the disc. The disc is called the *disc of convergence* and its radius is the *radius of convergence* of f(z) at $z = z_0$.

The next important notion is a geometric one.

DEFINITION IV.2. A function f(z) defined over a region Ω is called complex-differentiable (also holomorphic) at z_0 if the limit, for complex δz ,

$$\lim_{\delta z \to 0} \frac{f(z_0 + \delta z) - f(z_0)}{\delta z}$$

exists. (In particular, the limit is independent of the way δz tends to 0.) This limit is denoted as usual by $f'(z_0)$ or $\frac{d}{dz}f(z)|_{z_0}$ A function is complex-differentiable in Ω iff it is differentiable at every $z_0 \in \Omega$.

Clearly, if f(z) is complex differentiable at z_0 , it acts locally as a linear transformation,

$$f(z) - f(z_0) \sim f'(z_0)(z - z_0),$$

whenever $f'(z_0) \neq 0$. Then f(z) locally behaves like a similarity transformation (composed of a translation, a rotation, and a scaling). In particular, it preserves angles² and infinitesimal squares get transformed into infinitesimal squares; see Figure 3 for a rendering

²A mapping that preserves angles is also called a *conformal* map.



FIGURE 3. Multiple views of an analytic function. The image of the domain $\Omega = \{z \mid |\Re(z)| \leq 2, |\Im(z)| \leq 2\}$ by the function $f(z) = \exp(z) + z + 2$: (top) transformation of a square grid in Ω by f; (middle) the modulus and argument of f(z); (bottom) the real and imaginary parts of f(z).

It follows from a well known theorem of Riemann (see for instance [66, vol. 1, p 143]) that analyticity and complex differentiability are equivalent notions.

First fundamental property of analytic function theory. A function is analytic in a region Ω if and only if it is complex-differentiable in Ω .

 \triangleright 3. Analyticity implies complex-differentiability. Let f(z) be analytic at 0. Then its derivatives at a point z_0 within the disc of convergence of its expansion at 0 can be obtained by differentiating the

series representation of f termwise. Thus: *analytic implies complex-differentiable*. (The converse property requires integration properties and is discussed in Note 10 below.)

 \triangleright **4.** *Taylor's formula for analytic functions.* With the conventions of Note 3 and as a consequence of simple series rearrangements: *Taylor's formula holds at z*₀ *and one has*

$$f(z_0 + h) = \sum_{k=0}^{\infty} f^{(k)}(z_0) \frac{h^k}{k!}, \qquad f^{(k)}(z) = \frac{d^k}{dz^k} f(z).$$

for all small enough h.

 \triangleright 5. Cauchy–Riemann equations. Let $P(x, y) = \Re f(x + iy)$ and $Q(x, y) = \Im f(x + iy)$. By adopting successively in the definition of complex differentiability $\delta z = h$ and $\delta z = ih$, one finds

$$\frac{\partial P}{\partial x} + i\frac{\partial Q}{\partial x} = \frac{\partial Q}{\partial y} - i\frac{\partial P}{\partial y}$$

implying $P'_x = Q'_y$ and $P'_y = -Q'_x$, known as the Cauchy–Riemann equations. The functions P and Q satisfy the partial differential equations $\Delta f = 0$, where Δ is the 2-dimensional Laplacian $\Delta := \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2}$; such functions are known as harmonic functions.

We finally introduce meromorphic functions. The quotient of two analytic functions f(z)/g(z) ceases to be analytic at a point *a* where g(a) = 0. However, a simple structure for quotients of analytic functions prevails.

DEFINITION IV.3. A function h(z) is meromorphic at $z = z_0$ iff in a neighbourhood of $z = z_0$ with $z \neq z_0$ it is representable by an expansion of the form

(6)
$$h(z) = \sum_{n \ge -M} h_n (z - z_0)^n.$$

If $h_{-M} \neq 0$, then h(z) is said to have a pole of order M at z = a. The coefficient h_{-1} is called the residue of h(z) at z = a and is written as

$$\operatorname{Res}[h(z); z = a].$$

A function is meromorphic in a region iff it is meromorphic at any point of the region.

Equivalently, h(z) is meromorphic at $z = z_0$ iff, in a neighbourhood of z_0 , it can be represented as f(z)/g(z), with f(z) and g(z) being analytic at $z = z_0$.

IV.2.2. Integrals and residues. Integrals along curves in the complex plane are defined in the usual way from curvilinear integrals applied to the real and imaginary parts of the integrand. However integral calculus in the complex plane is of a radically different nature from what it is on the real line—in a way it is much simpler and much more powerful.

A path in a region Ω is described by its parameterization, which is a continuous function γ mapping [0, 1] into Ω . Two paths γ, γ' in Ω having the same end points are said to be *homotopic* (in Ω) if one can be continuously deformed into the other while staying within Ω as in the following examples:



A closed path is defined by the fact that its end points coincide: $\gamma(0) = \gamma(1)$, and a path is *simple* if the mapping γ is one-to-one. A closed path is said to be a *loop* of Ω if it can be continuously deformed *within* Ω to a single point; in this case one also says that the path is homotopic to 0. In what follows we implicitly restrict attention to paths that are assumed to be rectifiable. Unless otherwise stated, all integration paths will be assumed to be oriented positively.

One has:

Second fundamental property of analytic function theory. Let f be

analytic in Ω and let λ be a loop of Ω . Then $\int_{\lambda} f = 0$.

Equivalently, for f analytic in Ω , one has

(7)
$$\int_{\gamma} f = \int_{\gamma'} f,$$

provided γ and γ' are homotopic in γ .

 \triangleright **6.** *Proof of the Second Fundamental Principle from analyticity.* Let *f* be analytic in Ω . It suffices to justify

$$\int_{\lambda} \left[\sum_{n \ge 0} f_n z^n \right] dz = \sum_{n \ge 0} f_n \left[\int_{\lambda} z^n dz \right] = 0.$$

(The proof does not logically require the First Fundamental Principle.)

 \triangleright **7.** *Proof of the Second Fundamental Principle from differentiability.* Let *f* be complex-differentiable in Ω . Then the relation (7) holds. (The proof relies on the Cauchy–Riemann equations guaranteeing that the curvilinear integrals only depend on the endpoints of the contour; it does not logically require the First Fundamental Principle.) \triangleleft

The important *Residue Theorem* due to Cauchy relates *global* properties of a meromorphic function, its integral along closed curves, to purely *local* characteristics at designated points, the residues at poles.

THEOREM IV.1 (Cauchy's residue theorem). Let h(z) be meromorphic in the region Ω and let λ be a simple loop in Ω along which the function is analytic. Then

$$\frac{1}{2i\pi} \int_{\lambda} h(z) \, dz = \sum_{s} \operatorname{Res}[h(z); z = s],$$

where the sum is extended to all poles s of h(z) enclosed by λ .

PROOF. (Sketch) To see it in the representative case where h(z) has only a pole at z = 0, observe by appealing to primitive functions that

$$\int_{\lambda} h(z) dz = \sum_{\substack{n \ge -M \\ n \ne -1}} h_n \left[\frac{z^{n+1}}{n+1} \right]_{\lambda} + h_{-1} \int_{\lambda} \frac{dz}{z},$$

where the bracket notation $[u(z)]_{\lambda}$ designates the variation of the function u(z) along the contour λ . This expression reduces to its last term, itself equal to $2i\pi h_{-1}$, as is checked by using integration along a circle (set $z = re^{i\theta}$). The computation extends by translation to the case of a unique pole at z = a.

In the case of multiple poles, we observe that the simple loop can only enclose finitely many poles (by compactness). The proof then follows from a simple decomposition of the interior domain of λ into cells each containing only one pole. Here is an illustration

 \triangleleft



in the case of three poles. (Contributions from internal edges cancel.)

Here is a textbook example of such a reduction from global to local properties. Define the integrals

$$I_m := \int_{-\infty}^{\infty} \frac{dx}{1 + x^{2m}}$$

and consider specifically I_1 . Elementary calculus teaches us that $I_1 = \pi$ since the antiderivative of the integrand is an arc tangent:

$$I_1 = \int_{-\infty}^{\infty} \frac{dx}{1+x^2} = [\arctan x]_{-\infty}^{+\infty} = \pi.$$

In the light of the residue theorem, we first consider the integral over the whole line as the limit of integrals over large intervals of the form [-R, +R], then complete the contour of integration by means of a large semi-circle in the upper half-plane, as shown below:



Let γ be the contour comprised of the interval and the semi-circle. Inside γ , the integrand has a pole at x = i $(i = \sqrt{-1})$, where

$$\frac{1}{1+x^2} \equiv \frac{1}{(x+i)(x-i)} = -\frac{i}{2}\frac{1}{x-i} + \frac{1}{4} + \frac{i}{8}(x-i) + \cdots$$

so that its residue there is -i/2. Thus, by the residue theorem, the integral taken over γ is equal to $2\pi i$ times the residue of the integrand at i. As $R \to \infty$, the integral along the semi-circle vanishes (it is $O(R^{-1})$) while the integral along the real segment gives I_1 in the limit. There results the relation giving I_1 :

$$I_1 = 2i\pi \operatorname{Res}\left(\frac{1}{1+x^2}, x=i\right) = \pi$$

Remarkably, the evaluation of the integral in this perspective rests entirely upon the local expansion of the integrand at a special point (the point *i*).

 \triangleright 8. The general integral I_m . Let $\alpha = \exp(\frac{i\pi}{2m})$ so that $\alpha^{2m} = -1$. Contour integration of the type used for I_1 yields

$$I_m = 2i\pi \sum_{j=1}^m \text{Res}\left(\frac{1}{1+x^{2m}}; x = \alpha^{2j-1}\right),$$

while, for any $\beta = \alpha^{2j-1}$ with $1 \leq j \leq m,$ one has

$$\frac{1}{1+x^{2m}} \mathop{\sim}\limits_{x\to\beta} \frac{1}{2m\beta^{2m-1}} \frac{1}{x-\beta} \equiv -\frac{\beta}{2m} \frac{1}{x-\beta}$$

As a consequence,

$$I_{2m} = -\frac{i\pi}{m} \left(\alpha + \alpha^3 + \dots + \alpha^{2m-1} \right) = \frac{\pi}{m \sin \frac{\pi}{2m}}.$$

In particular, $I_2 = \pi/\sqrt{2}$, $I_3 = 2\pi/3$, $I_4 = \frac{\pi}{4}\sqrt{2}\sqrt{2+\sqrt{2}}$ as well as $\frac{1}{\pi}I_5$, $\frac{1}{\pi}I_6$ are expressible by radicals, but $\frac{1}{\pi}I_7$, $\frac{1}{\pi}I_9$ are not. The special cases $\frac{1}{\pi}I_{17}$, $\frac{1}{\pi}I_{257}$ are expressible by radicals.

> 9. Integrals of rational fractions. Generally, all integrals of rational functions taken over the whole real line are computable by residues. In particular,

$$J_m = \int_{-\infty}^{+\infty} \frac{dx}{(1+x^2)^m}, \qquad K_m = \int_{-\infty}^{+\infty} \frac{dx}{(1^2+x^2)(2^2+x^2)\cdots(m^2+x^2)}$$
explicitly evaluated.

can be explicitly evaluated.

Many function-theoretic consequences derive from the residue theorem. For instance, if f is analytic in Ω , $z_0 \in \Omega$ and λ is a simple loop of Ω encircling z_0 , one has

(8)
$$f(z_0) = \frac{1}{2i\pi} \int_{\lambda} f(\zeta) \frac{d\zeta}{\zeta - z_0}$$

This follows directly since

Res
$$[f(\zeta)(\zeta - z_0)^{-1}; \zeta = z_0] = f(z_0).$$

Then, by differentiation with respect to z under the integral sign, one gets similarly

(9)
$$\frac{1}{k!}f^{(k)}(z_0) = \frac{1}{2i\pi}\int_{\lambda} f(\zeta)\frac{d\zeta}{(\zeta - z_0)^k}.$$

The values of a function and its derivatives at a point can thus be obtained as values of integrals of the function away from that point.

A very important application of the residue theorem concerns coefficients of analytic functions.

THEOREM IV.2 (Cauchy's Coefficient Formula). Let f(z) be analytic in a region containing 0 and let λ be a simple loop around 0 that is oriented positively. Then the coefficient $[z^n]f(z)$ admits the integral representation

$$f_n \equiv [z^n]f(z) = \frac{1}{2i\pi} \int_{\lambda} f(z) \frac{dz}{z^{n+1}}.$$

PROOF. This formula follows directly from the equalities

$$\frac{1}{2i\pi} \int_{\lambda} f(z) \, \frac{dz}{z^{n+1}} = \operatorname{Res}\left[f(z)z^{-n-1}; z=0\right] = [z^n]f(z),$$

of which the first follows from the residue theorem, and the second from the identification of the residue at 0 as a coefficient. \square

▷ 10. Complex-differentiability implies analyticity. Formulæ (8) and (9) are by Note 5 consequences of complex-differentiability (without logically relying on the First Fundamental Principle). It is then a simple matter to complete the proof of the First Fundamental Property: one has (for h small enough)

$$f(z_{0}+h) = \frac{1}{2i\pi} \int_{\lambda} f(\zeta) \frac{d\zeta}{\zeta - (z_{0}+h)} \\ = \sum_{k \ge 0} \left[\frac{1}{2i\pi} \int_{\lambda} f(\zeta) \frac{d\zeta}{(\zeta - z_{0})^{k+1}} \right] h^{k} = \sum_{k \ge 0} f^{(k)}(z_{0}) \frac{h^{k}}{k!},$$

as results from expanding $(\zeta - z_0 - h)^{-1}$ into powers of h.

 \triangleleft

Analytically, the coefficient formula allows one to deduce information about the coefficients from the values of the function itself, using adequately chosen contours of integration. It thus opens the possibility of estimating the coefficients $[z^n]f(z)$ in the expansion of f(z) near 0 by using information on f(z) away from 0. The rest of this chapter will precisely illustrate this process in the case of functions whose singularities are poles, that is, rational and meromorphic functions. Note also that the residue theorem provides the simplest known proof of the Lagrange inversion theorem (see the appendices) whose rôle is *inter alia* central to tree enumerations. The supplements below explore some independent consequences of the residue theorem and the coefficient formula.

▷ 11. *Liouville's Theorem.* If a function f(z) is analytic in the whole of \mathbb{C} and is of modulus bounded by an absolute constant, $|f(z)| \leq B$, then it must be a constant. (By trivial bounds, upon integrating on a large circle, it is found that the Taylor coefficients at the origin of index ≥ 1 are all equal to 0.) Similarly, if f(z) is of at most polynomial growth, $|f(z)| \leq B (|z|+1)^r$ over the whole of \mathbb{C} , then it must be a polynomial.

 \triangleright 12. Lindelöf integrals. Let a(s) be analytic in $\Re(s) > \frac{1}{4}$ where it is assumed to satisfy $a(s) = O(\exp((\pi - \epsilon)|s|))$ for some $\epsilon > 0$. Then, one has for $\Re(z) > 0$,

$$\sum_{k=1}^{\infty} a(k)(-z)^k = -\frac{1}{2i\pi} \int_{1/2 - i\infty}^{1/2 + i\infty} a(s) z^s \frac{\pi}{\sin \pi s} \, ds$$

(Close the integration contour by a large semi-circle on the right.) Such integrals, sometimes called Lindelöf integrals, provide representations for functions determined by an explicit "law" of their Taylor coefficients [80].

As a consequence, the generalized polylogarithm functions

$$\operatorname{Li}_{\alpha,k}(z) = \sum_{n \ge 1} n^{-\alpha} (\log n)^k z^n$$

are analytic in the complex plane \mathbb{C} slit along $(1 + \infty)$. (More properties can be found in [39, 54].) For instance, one finds in this way

$$\sum_{n=1}^{\infty} (-1)^n \log n \, = -\frac{1}{8\pi} \int_{-\infty}^{+\infty} \frac{\log(\frac{1}{4} + t^2)}{\cosh(\pi t)} \, dt = 0.22579 \dots = \log\sqrt{\frac{\pi}{2}},$$

when the divergent series on the left is interpreted as $\operatorname{Li}_{0,1}(-1) = \lim_{z \to -1^+} \operatorname{Li}_{0,1}(z)$.

 \triangleright **13.** *Magic duality.* Let ϕ be a function initially defined over the nonnegative integers but admitting a meromorphic extension over the whole of \mathbb{C} . Under conditions analogous to those of Note 12, the function

$$F(z) := \sum_{n \ge 1} \phi(n) (-z)^n$$

which is analytic at the origin, is such that, near positive infinity,

$$F(z) \underset{z \to +\infty}{\sim} E(z) - \sum_{n \ge 1} \phi(-n)(-z)^{-n},$$

for some "elementary" function E(z). (Starting from the representation of Note 12, close the contour of integration by a large semicircle to the left.) In such cases, the function is said to satisfy the principle of *magic duality*—its expansion at 0 and ∞ are given by one and the same "law". Functions

$$\frac{1}{1+z}$$
, $\log(1+z)$, $\exp(-x)$, $\operatorname{Li}_2(-z)$, $\operatorname{Li}_3(-z)$

satisfy magic duality. Ramanujan [11] made a great use of this principle, which applies to a wide class of functions including hypergeometric ones; see [65, Ch XI] for an insightful discussion. \triangleleft

 \triangleright **14.** *Euler–Maclaurin and Abel–Plana summations.* Under simple conditions on the analytic function *f*, one has Plana's (also known as Abel's) complex variables version of the Euler–Maclaurin summation formula:

$$\sum_{n=0}^{\infty} f(n) = \frac{1}{2}f(0) + \int_{0}^{\infty} f(x) \, dx + \int_{0}^{\infty} \frac{f(iy) - f(-iy)}{e^{2i\pi y} - 1} \, dy.$$

(See [66, Vol. 1, p. 274] for a proof and validity conditions.)

 \triangleright 15. *Nörlund-Rice integrals*. Let a(z) be analytic for $\Re(z) > k_0 - \frac{1}{2}$ and of at most polynomial growth in this right half plane. Then, with γ a loop around the interval $[k_0, n]$, one has

$$\sum_{k=k_0}^n \binom{n}{k} (-1)^{n-k} a(k) = \frac{1}{2i\pi} \int_{\gamma} a(s) \frac{n! \, ds}{s(s-1)(s-2)\cdots(s-n)}$$

If a(z) is meromorphic in a larger region, then the integral can be estimated by residues. For instance, with

$$S_n = \sum_{k=1}^n \binom{n}{k} \frac{(-1)^k}{k}, \qquad T_n = \sum_{k=1}^n \binom{n}{k} \frac{(-1)^k}{k^2 + 1},$$

it is found that $S_n = -H_n$ (a harmonic number), while T_n oscillates boundedly as $n \to +\infty$. (This technique is a classical one in the calculus of finite differences, going back to Nörlund [87]. In computer science it is known as the method of "Rice's integrals" [50] and is used in the analysis of many algorithms and data structures including digital trees and radix sort [75, 108].)

IV. 3. Singularities and exponential growth of coefficients

For a given function, a singularity can be informally defined as a point where the function "ceases" to be analytic. Singularities are, as we have stressed repeatedly, essential to coefficient asymptotics. This section presents the bases of a discussion within the framework of analytic function theory.

IV.3.1. Singularities. Let f(z) be an analytic function defined over the interior region determined by a simple closed curve γ , and let z_0 be a point of the bounding curve γ . If there exists an analytic function $f^*(z)$ defined over some open set Ω^* containing z_0 and such that $f^*(z) = f(z)$ in $\Omega^* \cap \Omega$, one says that f is analytically continuable at z_0 and that f^* is an immediate analytic continuation of f.



In sharp contrast to real analysis where a function admits of many smooth extensions, analytic continuation is essentially *unique*: for instance, if f^* and f^{**} continue f at z_0 , then one must have $f^*(z) = f^{**}(z)$ in the vicinity of z_0 . Thus, the notion of immediate analytic continuation is intrinsic. Also the process can be iterated and we say that g is an *analytic continuation*³ of f, even if their domains of definition do not overlap, provided a finite chain of intermediate function elements connects f and g. This notion is once more intrinsic—this is known as the principle of *unicity of analytic continuation* (along paths).

 \triangleleft

³The collection of all function elements continuing a given function gives rise to the notion of Riemann surface, for which manty good books exist, e.g., [**33**, **105**]. We shall normally avoid appealing to this theory.

An analytic function is then much like a hologram: as soon as it is specified in any tiny region, it is rigidly determined in any wider region where it can be continued.

DEFINITION IV.4. Given an f defined in the region interior to γ , a point z_0 on the boundary of the region is a singular point or a singularity⁴ of f if f is not analytically continuable at z_0 .

Granted the intrinsic character of analytic continuation, we can usually dispense with a detailed description of the original domain Ω and the curve γ . In simple terms, a function is singular at z_0 if it cannot be continued as an analytic function beyond z_0 . A point at which a function is analytic is also called by contrast a *regular point*.

The two functions f(z) = 1/(1-z) and $g(z) = \sqrt{1-z}$ may be taken as initially defined over the open unit disk by their power series representation. Then, as we already know, they can be analytically continued to larger regions, the punctured plane $\Omega = \mathbb{C} \setminus \{1\}$ for f and the complex plane slit along $(1, +\infty)$ for g. (This is achieved by the usual operations of analysis, upon taking inverses and square roots.) But both are singular at 1: for f, this results from the fact that (say) $f(z) \to \infty$ as $z \to 1$; for g this is due to the branching character of the square-root.

It is easy to check from the definitions that a converging Taylor series is analytic inside its disc of convergence. In other words, it can have no singularity inside this disc. However, it *must* have one on the boundary of the disc, as asserted by the theorem below. In addition, a classical theorem, called Pringsheim's theorem [**109**, Sec. 7.21], provides a refinement of this property in the case of functions with nonnegative coefficients.

THEOREM IV.3 (Boundary singularities). (i) A function analytic f at the origin whose Taylor expansion at 0 has a finite radius of convergence R necessarily has a singularity on the boundary of its disc of convergence, |z| = R.

(*ii*) [Pringsheim's Theorem] If in addition f has nonnegative Taylor coefficients, then the point z = R is a singularity of f.

A figurative way of expressing Theorem IV.4, (i) is as follows:

The radius of convergence of a series equals its "radius of singularity".

(There "radius of singularity" means the first radius at which a singularity appears.) This result together with Pringsheim's is central to asymptotic enumeration as the remainder of this section will demonstrate.

PROOF. (i) Let f(z) be the function and R the radius of convergence of its Taylor series at 0, taken under the form

(10)
$$f(z) = \sum_{n \ge 0} f_n z^n.$$

We now that there can be no singularity of f within the disc |z| < R. Suppose a contrario that f(z) is analytic in the whole of $|z| < \rho$ for some ρ satisfying $\rho > R$. By Cauchy's coefficient formula (theorem IV.2), upon integrating along the circle λ of radius $r = (R + \rho)/2$, it is seen that the coefficient $[z^n]f(z)$ is $O(r^{-n})$. But then, the series expansion of f would have to converge in the disc of radius r > R, a contradiction. (More on this theme below.)

(*ii*) Suppose a contrario that f(z) is analytic at R, implying that it is analytic in a disc of radius r centred at R. We choose a number h such that $0 < h < \frac{1}{3}r$ and consider the

⁴For a detailed discussion, see [28, p. 229], [72, vol. 1, p. 82], or [109].

expansion of f(z) around $z_0 = R - h$:

(11)
$$f(z) = \sum_{m \ge 0} g_m (z - z_0)^m$$

By Taylor's formula and the representability of f(z) together with its derivatives at z_0 by means of (10), we have

$$g_m = \sum_{n \ge 0} \binom{n}{m} f_n z_0^m,$$

and in particular, $g_m \ge 0$. By the way h was chosen, the series (11) converges at $z - z_0 = 2h$, as illustrated by the following diagram:



Consequently, one has

$$f(R+h) = \sum_{m \ge 0} \left(\sum_{n \ge 0} \binom{n}{m} f_n z_0^{m-n} \right) (2h)^m.$$

This is a converging double sum of positive terms, so that the sum can be reorganized in any way we like. In particular, one has convergence of all the series involved in

$$f(R+h) = \sum_{m,n\geq 0} {n \choose m} f_n (R-h)^{m-n} (2h)^m$$

= $\sum_{n\geq 0} f_n [(R-h) + (2h)]^n$
= $\sum_{n\geq 0} f_n (R+h)^n.$

This establishes the fact that $f_n = o((R+h)^n)$, thereby reaching a contradiction. Pringsheim's theorem is proved.

Singularities of a function analytic at 0 which are on the boundary of the disc of convergence are called *dominant singularities*. The second part of this theorem appreciably simplifies the search for dominant singularities of combinatorial generating functions since these have nonnegative coefficients.

For instance, the derangement OGF and the surjection EGF,

$$D(z) = \frac{e^{-z}}{1-z}, \qquad S(z) = (2-e^z)^{-1}$$

are analytic except for a simple pole at z = 1 in the case of D(z), and except for points $z_k = \log 2 + 2ik\pi$ that are simple poles in the case of S(z). Thus the dominant singularities for derangements and surjections are at 1 and $\log 2$ respectively.



FIGURE 4. The images of a grid on the unit square (with corners $\pm 1 \pm i$) by various functions singular at z = 1 reflect the nature of the singularities involved. Here (from top to bottom) $f_0(z) = 1/(1-z)$, $f_1(z) = \exp(z/(1-z))$, $f_2(z) = -(1-z)^{1/2}$, $f_3(z) = -(1-z)^{3/2}$, $f_4(z) = \log(1/(1-z))$. The functions have been normalized to be increasing over the real interval [-1, 1]. Singularities are apparent near the right of each diagram where small grid squares get folded or unfolded in various ways. (In the case of functions f_0, f_1, f_4 that become infinite at z = 1, the grid has been slightly truncated to the right.)

It is known that \sqrt{Z} cannot be unambiguously defined as an analytic function in a neighbourhood of Z = 0. As a consequence, the function

$$C(z) = (1 - \sqrt{1 - 4z})/2$$

which is the generating function of the Catalan numbers, is an analytic function in certain regions that should exclude 1/4; for instance, one may opt to take the complex plane slit along the ray $(1/4, +\infty)$. Similarly, the function

$$L(z) = \log \frac{1}{1-z}$$

which is the EGF of cyclic permutations is analytic in the complex plane slit along $(1, +\infty)$. (An alternative way of seeing that C(z) and L(z) are singular at $\frac{1}{4}$ and 1 is to observe that their derivatives become infinite along rays $z \to \frac{1}{4}^-$ and $z \to 1^-$.)

A function having no singularity at a finite distance is called *entire*; its Taylor series then converges everywhere in the complex plane. The EGFs,

$$e^{z+z^2/2}, e^{e^z-1},$$

associated to involutions and set partitions are entire.

IV.3.2. The Exponential Growth Formula. We say that a number sequence $\{a_n\}$ is of *exponential order* K^n which we abbreviate as (the symbol \bowtie is a "bowtie")

$$a_n \bowtie K^n$$
 iff $\limsup |a_n|^{1/n} = K.$

The relation $X \bowtie Y$ reads as "X is of exponential order Y". In other words, for any $\epsilon > 0$:

 $|a_n| >_{i.o} (K - \epsilon)^n$, that is to say, $|a_n|$ exceeds $(K - \epsilon)^n$ infinitely often (for infinitely many values of n);

 $|a_n| <_{a.e.} (K + \epsilon)^n$, that is to say, $|a_n|$ is dominated by $(K + \epsilon)^n$ almost everywhere (except for possibly finitely many values of n).

This relation can be rephrased as $a_n = \vartheta(n)K^n$, where ϑ is a *subexponential factor* satisfying

$$\limsup |\theta(n)|^{1/n} = 1;$$

such a factor is thus bounded from above almost everywhere by any increasing exponential (of the form $(1+\epsilon)^n$) and bounded from below infinitely often by any decaying exponential (of the form $(1-\epsilon)^n$). Typical subexponential factors are

1,
$$n^3$$
, $(\log n)^2$, \sqrt{n} , $\frac{1}{\sqrt[3]{\log n}}$, $n^{-3/2}$, $\log \log n$.

(Note that functions like $e^{\sqrt{n}}$ and $\exp(\log^2 n)$ must be treated as subexponential factors for the purpose of this discussion.) In this and the next chapters, we shall see general methods that enable one to extract such subexponential factors from generating functions.

THEOREM IV.4 (Exponential Growth Formula). If f(z) is analytic at 0 and R is the modulus of a singularity of f(z) nearest to the origin,

$$R = \min\{ |z|, z \in \operatorname{Sing}(f) \},\$$

then the coefficient $f_n = [z^n]f(z)$ satisfies

$$f_n \bowtie \left(\frac{1}{R}\right)^n$$
, equivalently $f_n = \left(\frac{1}{R}\right)^n \theta(n)$ with $\limsup |\theta(n)|^{1/n} = 1$.

PROOF. The lower bound follows since otherwise the series would converge (and hence be analytic) in a larger domain. Trivial bounds on Cauchy's coefficient formula upon taking as contour λ a circle of radius $R - \eta$,

$$|f_n| \leq \frac{1}{2\pi} \frac{\max\{|f(z)|/|z| = R - \eta\}}{|R - \eta|^{n+1}} \cdot (2\pi R)$$

$$\leq \mathcal{O}((R - \eta)^{-n}),$$

yield the upper bound.

The exponential growth formula thus directly relates the exponential order of growth of coefficients of a function to the *location* of its singularities nearest to the origin. Several direct applications to combinatorial enumeration are given below.

EXAMPLE 1. *Exponential growth and combinatorial enumeration*. Here are a few immediate applications of of exponential bounds to surjections, derangements, integer partitions, and unary binary trees.

Surjections. The function

$$R(z) = (2 - e^z)^{-1}$$

is the EGF of surjections. The denominator is an entire function, so that singularities may only arise from its zeros, to be found at the points

$$\chi_k = \log 2 + 2ik\pi, \qquad k \in \mathbb{Z}$$

The dominant singularity of R is then at $\rho = \chi_0 = \log 2$. Thus, with $r_n = [z^n]R(z)$,

$$r_n \bowtie (\frac{1}{\log 2})^n.$$

Similarly, if "double" surjections are considered (each value in the range of the surjection is taken at least twice), the corresponding EGF is

$$R^*(z) = \frac{1}{2 - z - e^z};$$

the dominant singularity is at ρ^* defined as the positive root of equation $e^{\rho^*} - \rho^* = 2$, and the coefficient r_n^* satisfies: $r_n^* \bowtie (\frac{1}{\rho^*})^n$ Numerically, this gives

$$r_n \bowtie 1.44269^n$$
 and $r_n^* \bowtie 0.87245^n$,

with the actual figures for the corresponding logarithms being

n	$\frac{1}{n}\log r_n$	$\frac{1}{n}\log r_n^*$
10	0.33385	0.80208
20	0.35018	0.80830
50	0.35998	0.81202
100	0.36325	0.81327
∞	0.36651	0.81451
	$(\log 1/\rho)$	$(\log(1/ ho^*)$

These estimates constitutes a weak form of a more precise result to be established later in this chapter: If random surjections of size n are taken equally likely, the probability of a surjection being a double surjection is exponentially small.

Derangements. There, for $d_{1,n} = [z^n]e^{-z}(1-z)^{-1}$ and $d_{2,n} = [z^n]e^{-z-z^2/2}(1-z)^{-1}$ we have, from the poles at z = 1,

$$d_{1,n} \bowtie 1^n$$
 and $d_{2,n} \bowtie 1^n$

The upper bound is combinatorially trivial. The lower bound expresses that the probability for a random permutation to be a derangement is *not* exponentially small. For $d_{1,n}$, we have already proved by an elementary argument the stronger result $d_{1,n} \rightarrow e^{-1}$; in the case of $d_{2,n}$, we shall establish later the precise asymptotic equivalent $d_{2,n} \rightarrow e^{-3/2}$, in accordance with what was announced in the introduction.

Unary-Binary trees. The expression

$$U(z) = \frac{1 - z - \sqrt{1 - 2z - 3z^2}}{2z} = z + z^2 + 2z^3 + 4z^4 + 9z^5 + \cdots,$$

represents the OGF of (plane unlabelled) unary-binary trees. From the equivalent form,

$$U(z) = \frac{1 - z - \sqrt{(1 - 3z)(1 + z)}}{2z},$$

it follows that U(z) is analytic in the complex plane slit along $(\frac{1}{3}, +\infty)$ and $(-\infty, -1)$ and is singular at z = -1 and z = 1/3 where it has branch points. The closest singularity to the origin being at $\frac{1}{3}$, one has

 $U_n \bowtie 3^n$.

In this case, the stronger upper bound $U_n \leq 3^n$ results directly from the possibility of encoding such trees by words over a ternary alphabet using Łukasiewicz codes (Chapter I). A complete asymptotic expansion will be obtained in the next chapter.

The exponential growth formula expressed by Theorem IV.4 can be supplemented by effective upper bounds which are very easy to derive and often turn out to be surprisingly accurate. We state:

PROPOSITION IV.1 (Saddle-Point bounds). Let f(z) be analytic in the disc |z| < Rwith $0 < R \le \infty$. Then, one has, for any r in (0, R), the family of saddle point upper bounds (12)

$$[z^{n}]f(z) \leq \frac{\sup_{|z|=r} |f(z)|}{r^{n}} \quad (any r), \quad and \quad [z^{n}]f(z) \leq \inf_{s \in (0,R)} \frac{\sup_{|z|=s} |f(z)|}{s^{n}}$$

If in addition f(z) has nonnegative coefficients at 0, then

(13)
$$[z^n]f(z) \leq \frac{f(r)}{r^n}$$
 (any r), and $[z^n]f(z) \leq \inf_{s \in (0,R)} \frac{f(s)}{s^n}$.

PROOF. The first bound in (12) results from trivial bounds applied to the Cauchy coefficient formula, when integration is performed along a circle. It is consequently valid for any r smaller than the radius of convergence of f at 0. The best possible such bound is then given by the second inequality; it can be determined by cancelling a derivative,

$$s : s \frac{f'(s)}{f(s)} = n.$$

Note that because of the first inequality, any approximate solution of this last equation will in fact provide a valid upper bound.

The bounds (13) can be viewed as a specialization of (12). Alternatively, they can be obtained elementarily since

$$f_n \le \frac{f_0}{r^n} + \dots + \frac{f_{n-1}}{r^{n-1}} + f_n + \frac{f_{n+1}}{r^{n+1}} + \dots,$$

whenever the f_k are nonnegative.

n	\widetilde{I}_n	I_n
100	$0.106579 \cdot 10^{85}$	$0.240533 \cdot 10^{83}$
200	$0.231809 \cdot 10^{195}$	$0.367247 \cdot 10^{193}$
300	$0.383502 \cdot 10^{316}$	$0.494575\cdot 10^{314}$
400	$0.869362 \cdot 10^{444}$	$0.968454\cdot 10^{442}$
500	$0.425391 \cdot 10^{578}$	$0.423108 \cdot 10^{576}$



FIGURE 5. The comparison between the exact number of involutions I_n and its approximation $\tilde{I}_n = n! e^{\sqrt{n} + n/2} n^{-n/2}$: (left) a table; (right) a plot of $\log_{10}(I_n/\tilde{I}_n)$ against $\log_{10} n$ suggesting that the ratio is $\sim K \cdot n^{-1/2}$.

For reasons well explained by the saddle point method (Chapter VI), these bounds usually capture the actual asymptotic behaviour up to a polynomial factor only. A typical instance is the weak form of Stirling's formula,

$$\frac{1}{n!} \equiv [z^n]e^z \le \frac{e^n}{n^n},$$

which only overestimates the true asymptotic value by a factor of $\sqrt{2\pi n}$.

EXAMPLE 2. *Combinatorial examples of saddle point bounds*. Here are applications to fragmented permutations, set partitions (Bell numbers), involutions, and integer partitions.

Fragmented permutations. Consider first the EGF of "fragmented permutations" (Chapter II) defined by $\mathcal{F} = \mathfrak{P}(\mathfrak{S}_{\geq 1}(\ddagger))$ in the labelled universe. We claim that

(14)
$$\frac{1}{n!}F_n \equiv [z^n]e^{z/(1-z)} \le e^{2\sqrt{n}-\frac{1}{2}+O(n^{-1/2})}.$$

Indeed, the minimizing value of r in (13) is r_0 such that

$$0 = \frac{d}{dr} \left(\frac{r}{1-r} - n \log r \right)_{r=r_0} = \frac{1}{(1-r_0)^2} - \frac{n}{r_0}.$$

The equation is solved by $r_0 = (2n + 1 - \sqrt{4n + 1})/(2n)$. One can either use this exact value and perform asymptotic approximation of $f(r_0)/z_0^n$, or adopt the approximate value $r_1 = 1 - 1/\sqrt{n}$, which leads to simpler calculations. The estimate (14) results.

Bell numbers and set partitions. Another immediate applications is an upper bound on Bell numbers enumerating set partitions with EGF e^{e^z-1} . The best saddle point bound is

(15)
$$\frac{1}{n!}B_n \le e^{e^r - 1 - n\log r}, \qquad r : re^r = n,$$

with $r \sim \log n - \log \log n$.

Involutions. Regarding involutions, their EGF is $I(z) = \exp(z + \frac{1}{2}z^2)$, and one determines (see Figure 5 for numerical data)

(16)
$$\frac{1}{n!}I_n \le \frac{e^{\sqrt{n}+n/2}}{n^{n/2}}$$

Similar bounds hold for permutations with all cycle lengths $\leq k$ and permutations σ such that $\sigma^k = Id$.

Integer partitions. The function

(17)
$$P(z) = \prod_{k=1}^{\infty} \frac{1}{1-z^k} = \exp\left(\sum_{\ell=1}^{\infty} \frac{1}{\ell} \frac{z^\ell}{1-z^\ell}\right)$$

is the OGF of integer partitions, the unlabelled analogue of set partitions. Its radius of convergence is *a priori* bounded from above by 1, since the set \mathcal{P} is infinite and the second form of P(z) shows that it is exactly equal to 1. Therefore $P_n \bowtie 1^n$. A finer upper bound results from the estimate

(18)
$$\Lambda(t) := \log P(e^{-t}) \sim \frac{\pi^2}{6t} + \log \sqrt{\frac{t}{2\pi}} - \frac{1}{24}t + O(t^2),$$

which obtains from Euler–Maclaurin summation or, better, from a Mellin analysis following APPENDIX: *Mellin transform*, p. 120. Indeed, the Mellin transform of Λ is, by the harmonic sum rule,

$$\Lambda^{\star}(s) = \zeta(s)\zeta(s+1)\Gamma(s), \qquad s \in \langle 1, +\infty \rangle,$$

and the successive leftmost poles at s = 1 (simple pole), s = 0 (double pole), and s = -1 (simple pole) translate into the asymptotic expansion (18). When $z \to 1^-$, this means that

(19)
$$P(z) \sim \frac{e^{-\pi^2/12}}{\sqrt{2\pi}} \sqrt{1-z} \exp\left(\frac{\pi^2}{6(1-z)}\right),$$

from which we derive the upper bound,

$$P_n \le C n^{1/4} e^{\pi \sqrt{2n/3}}$$

(for some C > 0) in a way analogous to fragmented permutations above. This last bound loses only a polynomial factor, as we shall prove when studying the saddle point method in Chapter VIII.

 \triangleright 16. A natural boundary. One has $P(re^{i\theta}) \to \infty$ as $r \to 1^-$, for any angle θ that is a rational multiple of 2π . Such points being dense on the unit circle, the function P(z) admits the unit circle as a *natural boundary*, i.e., it cannot be analytically continued beyond this circle.

 \triangleright 17. *Meinardus' method.* The combination of Mellin transforms and saddle point analysis in the theory of partitions is known as Meinardus' method [4, Ch. 6]. Consider the set \mathcal{R} of compositions into *r*th powers ($r \ge 2$). The OGF satisfies

$$\Lambda(t) := \log R(e^{-t}) = \sum_{\ell \ge 1} \frac{1}{\ell} \frac{e^{-\ell^r t}}{1 - e^{-\ell^r t}};$$

with Mellin transform $\Lambda^*(s) = \zeta(rs)\zeta(s+1)\Gamma(s)$ defined for $\Re(s) > r^{-1}$. From the pole of Λ^* at s = 1/r, one gets

$$R(z) = \exp\left(\frac{\xi}{(1-z)^{1/r}}\right) (1+o(1)), \qquad \xi := \frac{1}{r}\zeta(1+\frac{1}{r})\Gamma(\frac{1}{r}).$$

The minimizing value s_0 for saddle point bounds satisfies $1 - s_0 (rn/\xi)^{-r/(r+1)}$, and

$$\log R_n \le Cn^{\frac{1}{r+1}}(1+o(1))$$

(for some C > 0). See Andrews' book [4, Ch. 6] for precise asymptotics and a general setting.

IV.3.3. Closure properties and computable bounds. The functions analytic at a point z = a are closed under sum and product, and hence form a ring. If f(z) and g(z) are analytic at z = a, then so is their quotient f(z)/g(z) provided $g(a) \neq 0$. Meromorphic functions are furthermore closed under quotient and hence form a field. Such properties are proved most easily using complex-differentiability and extending the usual relations from real analysis, (f + g)' = f' + g', (fg)' = fg' = f'g, and so on.

Analytic functions are also closed under composition: if f(z) is analytic at z = a and g(w) is analytic at b = f(a), then $g \circ f(z)$ is analytic at z = a. Graphically:



The proof based on complex-differentiability closely mimicks the real case. Inverse functions exist conditionally: if $f'(a) \neq 0$, then f(z) is locally linear near a, hence invertible, so that there exists a g satisfying $f \circ g = g \circ f = Id$, where Id is the identity function, $Id(z) \equiv z$. The inverse function is itself locally linear, hence complex differentiable, hence analytic. In short, the inverse of an analytic function f at a place where its derivative does not vanish is an analytic function.

One way to establish closure properties, as suggested above, is to deduce analyticity criteria from complex differentiability by way of the "First Fundamental Property". An alternative approach, closer to the original notion of analyticity, can be based on a two-step process: (i) closure properties are shown to hold true for formal power series; (ii) the resulting formal power series are proved to be locally convergent by means of suitable majorizations on their coefficients. This is the basis of the classical method of *majorant series* originating with Cauchy.

▷ 18. The majorant series technique. Given two power series, define $f(z) \leq g(z)$ if $|[z^n]f(z)| \leq [z^n]g(z)$ for all $n \geq 0$. The following two conditions are equivalent: (i) f(z) is analytic in the disc $|z| < \rho$; (ii) for any $r < \rho$ there exists a *c* such that

$$f(z) \preceq \frac{c}{1 - rz}$$

If f, g are majorized by c/(1-rz), d/(1-rz) respectively, then f + g and $f \cdot g$ are majorized,

$$f(z) + g(z) \preceq \frac{c+d}{1-rz}, \qquad f(z) \cdot g(z) \preceq \frac{e}{1-sz},$$

for any s < r and some e dependent on s. If f, g are majorized by c/(1 - rz), dz/(1 - rz) respectively, then $f \circ g$ is majorized:

$$f \circ g(z) \preceq \frac{cz}{1 - r(1 + d)z}.$$

Constructions for 1/f and for the functional inverse of f can be similarly developed. See Cartan's book [17] and van der Hoeven's study [110] for a systematic treatment.

For functions defined by analytic expressions, singularities can be determined inductively in an intuitively transparent manner. If Sing(f) and Zero(f) are the set of singularities and zeros of function f, then, due to closure properties of analytic functions, the following informally stated guidelines apply.

$\operatorname{Sing}(f \pm g)$	\subseteq	$\operatorname{Sing}(f) \cup \operatorname{Sing}(g)$
$\operatorname{Sing}(f \times g)$	\subseteq	$\operatorname{Sing}(f) \cup \operatorname{Sing}(g)$
$\operatorname{Sing}(f/g)$	\subseteq	$\operatorname{Sing}(f) \cup \operatorname{Sing}(g) \cup \operatorname{Zero}(g)$
$\operatorname{Sing}(f \circ g)$	\subseteq	$\operatorname{Sing}(g) \cup g^{(-1)}(\operatorname{Sing}(f))$
$\operatorname{Sing}(\sqrt{f})$	\subseteq	$\operatorname{Sing}(f) \cup \operatorname{Zero}(f)$
$\operatorname{Sing}(\log(f))$	\subseteq	$\operatorname{Sing}(f) \cup \operatorname{Zero}(f)$
$\operatorname{Sing}(f^{(-1)})$	\subseteq	$f(\operatorname{Sing}(f)) \cup f(\operatorname{Zero}(f')).$

A mathematically rigorous treatment would require considering multivalued functions and Riemann surfaces, so that we do not state detailed validity conditions and, at this stage, keep for these formulæ the status of useful heuristics. In fact, because of Pringsheim's theorem, the search of dominant singularities of combinatorial generating function can normally avoid considering the multivalued structure of functions, since only some initial segment of the positive real half–line needs to be considered. This in turn implies a powerful and easy way of determining the exponential order of coefficients of a wide variety of generating functions, as we now explain.

As defined in Chapters I and II, a combinatorial class is *constructible* if it can be specified by a finite set of equations involving only basic constructors. A specification is *iterative* if the dependency graph of the specification is acyclic, that is, no recursion is involved and a single functional term (written with sums, products, as well as sequence, set, and cycle constructions) describes the specification. We state:

THEOREM IV.5 (Computability of growth). Let C be a constructible unlabelled class that admits of an iterative specification in terms of $(1, \mathcal{Z}; \mathfrak{S}, \mathfrak{P}, \mathfrak{M}, \mathfrak{C}; +, \times)$. Then the radius of convergence ρ_C of the OGF C(z) of C is a nonzero computable real number.

Let \mathcal{D} be a constructible labelled class that admits of an iterative specification in terms of $(1, \mathcal{Z}; \mathfrak{S}, \mathfrak{P}, \mathfrak{C}; +, \star)$. Then the radius of convergence ρ_D of the EGF D(z) of \mathcal{D} is a nonzero computable real number.

Accordingly, the exponential rate of growth of the coefficients $[z^n]C(z)$ and $[z^n]D(z)$ are computable real numbers.

A real number α is computable iff there exists a program Π_{α} which on input *m* outputs a rational number α_m that is within $\pm 10^{-m}$ of α . The theorem immediately implies that the exponential growth estimates,

$$[z^n]C(z) \equiv C_n \bowtie \left(\frac{1}{\rho_C}\right)^n, \qquad [z^n]D(z) \equiv \frac{1}{n!}D_n \bowtie \left(\frac{1}{\rho_D}\right)^n,$$

for coefficients are automatically computable from the specification itself.

PROOF. In both cases, the proof proceeds by induction on the structural specification of the class. For each class \mathcal{F} , with generating function F(z), we associate a *signature*, which is an ordered pair $\langle \rho_F, \tau_F \rangle$, where ρ_F is the radius of convergence of F and τ_F is the value of F at ρ_F , precisely,

$$\tau_F := \lim_{x \to \rho_F^-} F(x).$$

(The value τ_F is well defined as an element of $\mathbb{R} \cup \{+\infty\}$ since F, being a counting generating function, is necessarily increasing on $(0, \rho_F)$.) We prove the assertion of the theorem together with the additional property that $\tau_F = \infty$ and as soon as one of the unary constructors $(\mathfrak{S}, \mathfrak{M}, \mathfrak{P}, \mathfrak{C})$ intervenes in the specification, that is, as soon as the class is infinite. In that case, since the OGF includes infinitely many terms of the form z^n , it must be divergent at 1, so that $\rho_F \leq 1$ holds *a priori* for all infinite classes under consideration.

Consider the unlabelled case first. The signatures of the neutral class 1 and the atomic class \mathcal{Z} , with OGF 1 and z, are $\langle +\infty, 1 \rangle$ and $\langle +\infty, +\infty \rangle$. Any nonconstant polynomial which is the OGF of a finite set has the signature $\langle +\infty, +\infty \rangle$. The assertion is thus easily verified in these cases.

Next, let $\mathcal{F} = \mathfrak{S}(\mathcal{G})$. The OGF G(z) must be nonconstant and in fact satisfy G(0) = 0in order for the sequence construction to be properly defined. Thus, by the induction hypothesis, one has $0 < \rho_G \leq +\infty$ and $\tau_G = +\infty$. Now, the function G being increasing and continuous along the positive axis, there must exist a value β such that $0 < \beta < \rho_G$ with $G(\beta) = 1$. For $z \in (0, \beta)$, the quasi-inverse $F(z) = (1 - G(z))^{-1}$ is well defined and analytic; as z approaches β from the left, F(z) increases unboundedly. Thus, the smallest singularity of F along the positive axis is at β , and by Pringsheim's theorem, one has $\rho_F = \beta$. The argument also shows that $\tau_F = +\infty$. There only remains to check that β is computable. The coefficients of G form a computable sequence of integers, so that G(x), which can be well approximated via truncated Taylor series, is an effectively computable number⁵ if x is itself a positive computable number less than ρ_G . Then dichotomic search constitutes effectively an algorithm for determining β .

Next, we consider the multiset construction, $\mathcal{F} = \mathfrak{M}(\mathcal{G})$, whose translation into OGFs necessitates the "Pólya exponential":

$$F(z) = \operatorname{Exp}(G(z))$$
 where $\operatorname{Exp}(h(z)) := \exp\left(h(z) + \frac{1}{2}h(z^2) + \frac{1}{3}h(z^3) + \cdots\right)$.

Once more, the induction hypothesis is assumed for G. If G is polynomial, then F is a variant of the OGF of integer partitions, and in fact is expressible as a finite product of terms of the form $P(z), P(z^2), P(z^3), \ldots$ Thus, $\rho_F = 1$ and $\tau_F = \infty$ in that particular case. In the general case of $\mathcal{F} = \mathfrak{M}(\mathcal{G})$ with \mathcal{G} infinite, we start by fixing arbitrarily a number r such that $0 < r < \rho_G \le 1$ and examine F(z) for $z \in (0, r)$. The expression for F rewrites as

$$\operatorname{Exp}(G(z)) = e^{G(z)} \cdot \exp\left(\frac{1}{2}G(z^2) + \frac{1}{3}G(z^3) + \cdots\right).$$

The first factor is analytic for z on $(0, \rho_G)$ since, the exponential function being entire, e^G has the singularities of G. As to the second factor, one has G(0) = 0 (in order for the set construction to be well-defined), while G(x) is convex for $x \in [0, r]$ (since its second derivative is positive). Thus, there exists a positive constant K such that $G(x) \leq Kx$ when $x \in [0, r]$. Then, the series $\frac{1}{2}G(z^2) + \frac{1}{3}G(z^3) + \cdots$ has its terms dominated by those of the convergent series

$$\frac{K}{2}r^2 + \frac{K}{3}r^3 + \dots = K\log(1-r)^{-1} - Kr.$$

By a well known theorem of analytic function theory, a uniformly convergent sum of analytic functions is itself analytic; consequently, $\frac{1}{2}G(z^2) + \frac{1}{3}G(z^3) + \cdots$ is analytic at all z of (0, r). Analyticity is then preserved by the exponential, so that F(z), being analytic at $z \in (0, r)$ for any $r < \rho_G$ has a radius of convergence that satisfies $\rho_F \ge \rho_G$. On the other hand, since F(z) dominates termwise G(z), one has $\rho_F \le \rho_G$. Thus finally one has $\rho_F = \rho_G$. Also, $\tau_G = +\infty$ implies $\tau_F = +\infty$.

A completely parallel discussion covers the case of the powerset construction (\mathfrak{P}) whose associated functional $\overline{\text{Exp}}$ is a minor modification of the Pólya exponential Exp.

⁵The present argument only establishes non-constructively the *existence* of a program, based on the fact that truncated Taylor series converge geometrically fast at an interior point of their disc of convergence. Making explicit this program and the involved parameters however represents a harder problem that is not touched upon here.



FIGURE 6. A random train.

The cycle construction can be treated by similar arguments based on consideration of "Pólya's logarithm" as $\mathcal{F} = \mathfrak{C}(\mathcal{G})$ corresponds to

$$F(z) = \text{Log} \frac{1}{1 - G(z)}$$
, where $\text{Log} h(z) = \log h(z) + \frac{1}{2} \log h(z^2) + \cdots$.

In order to conclude with the unlabelled case, there only remains to discuss the binary constructors +, ×, which give rise to F = G + H, $F = G \cdot H$. It is easily verified that $\rho_F = \min(\rho_G, \rho_H)$ and $\tau_F = \tau_G \circ \tau_H$ with \circ being + or ×. Computability is granted since the minimum of two computable numbers is computable.

The labelled case is covered by the same type of argument as above. The discussion is even simpler, since the ordinary exponential and logarithm replace the Pólya operators Exp and Log. It is still a fact that all the EGFs of infinite families are infinite at their dominant positive singularity, though the radii of convergence can now be of any magnitude (w.r.t. 1).

▷ **19.** Syntactically decidable properties. In the unlabelled case, $\rho_F = 1$ iff the specification of \mathcal{F} only involves $(1, \mathcal{Z}; \mathfrak{P}, \mathfrak{M}; +, \times)$ and at least one of $\mathfrak{P}, \mathfrak{M}$.

▷ 20. Nonconstructibility of permutations and graphs. The class \mathcal{P} of all permutations cannot be specified as a constructible unlabeled class since the OGF $P(z) = \sum_n n! z^n$ has radius of convergence 0. (It is of course constructible as a labelled class.) Graphs, whether labelled or unlabelled, are too numerous to form a constructible class.

Theorem IV.5 establishes a link between analytic combinatorics, computability theory, and symbolic manipulation systems. It is based on an article of Flajolet, Salvy, and Zimmermann [49] devoted to such computability issues in exact and asymptotic enumeration. Recursive specifications are not discussed now since they tend to give rise to branch points, themselves amenable to singularity analysis techniques to be developed in the next chapter.

EXAMPLE 3. *Combinatorial trains*. This somewhat artificial example from [**38**] serves to illustrate the scope of Theorem IV.5 and demonstrate its inner mechanisms at work. Define the class of all labelled trains by the following specification,

(20)
$$\begin{cases} \mathcal{T} = \mathcal{W}a \star \mathfrak{S}(\mathcal{W}a \star \mathfrak{P}(\mathcal{P}a)), \\ \mathcal{W}a = \mathfrak{S}_{\geq 1}(\mathcal{P}\ell), \\ \mathcal{P}\ell = \mathcal{Z} \star \mathcal{Z} \star (\mathbf{1} + \mathfrak{C}(\mathcal{Z})), \\ \mathcal{P}a = \mathfrak{C}(\mathcal{Z}) \star \mathfrak{C}(\mathcal{Z}). \end{cases}$$



FIGURE 7. The inductive determination of the radius of convergence of the EGF of trains, T(z): (top) a hierarchical view of the specification of \mathcal{T} ; (bottom left) the corresponding expression tree of the EGF T(z); (bottom right) the value of the radii for each subexpression of T(z). (Notations: $L(y) = \log(1-y)^{-1}$, $S(y) = (1-y)^{-1}$, $S_1(y) = yS(y)$.)

In figurative terms, a train (\mathcal{T}) is composed of a first wagon ($\mathcal{W}a$) to which is appended a sequence of passenger wagons, each of the latter capable of containing a set of passengers ($\mathcal{P}a$). A wagon is itself composed of "planks" ($\mathcal{P}\ell$) determined by their end points ($\mathcal{Z} \star \mathcal{Z}$) and to which a circular wheel ($\mathfrak{C}(\mathcal{Z})$) may be attached. A passenger is composed of a head and a belly that are each circular arrangements of atoms (see Figure 6).

The translation into a set of EGF equations is immediate and a symbolic manipulation system readily provides the form of the EGF of trains, T(z), as

$$T(z) = \frac{z^2 \left(1 + \log((1-z)^{-1})\right)}{\left(1 - z^2 \left(1 + \log((1-z)^{-1})\right)\right)} \left(1 - \frac{z^2 \left(1 + \log((1-z)^{-1})\right) e^{\left(\log((1-z)^{-1})\right)^2}}{1 - z^2 \left(1 + \log((1-z)^{-1})\right)}\right)^{-1},$$

together with the expansion

$$T(z) = 2\frac{z^2}{2!} + 6\frac{z^3}{3!} + 60\frac{z^4}{4!} + 520\frac{z^5}{5!} + 6660\frac{z^6}{6!} + 93408\frac{z^7}{7!} + \cdots$$

The specification (20) has a hierarchical structure, as suggested by the top representation of Figure 7, and this structure is itself directly reflected by the form of the expression tree of the GF T(z). Then each node in the expression tree of T(z) can be tagged with the corresponding value of the radius of convergence. This is done according to the principles of Theorem IV.5; see the bottom-right part of Figure 7. For instance, the quantity 0.68245 associated to Wa(z) is given by the sequence rule and is determined as smallest positive solution to the equation

$$z^{2} \left(1 - \log(1 - z)^{-1}\right) = 1$$

The tagging process works upwards till the root of the tree is reached; here the radius of convergence of T is determined to be $\rho \doteq 0.48512\cdots$, a quantity that happens to coincide with the ratio $[z^{49}]T(z)/[z^{50}]T(z)$ to more than 15 decimal places.

IV.4. Rational and meromorphic functions

The first principle that we have just discussed in great detail is:

The location of singularities of an analytic function determines the exponential order of growth of its Taylor coefficients.

The second principle which refines the first one is:

The nature of the singularities determines the way the dominant exponential term in coefficients is modulated by a subexponential factor.

We are now going to develop the correspondence between singular expansions and asymptotic behaviours of coefficients in the case of rational and meromorphic functions. Rational functions (fractions) are the simpler ones, and from their basic partial fraction expansion closed forms are derived for their coefficients. Next in order of difficulty comes the class of meromorphic functions; their Taylor coefficients appear to admit very accurate asymptotic expansions with error terms that are exponentially small, as results from an adequate use of the residue theore.

In the case of rational and, more generally, meromorphic functions, the net effect is summarized by the correspondence:

Polar singularities \rightsquigarrow Subexponential factors $\theta(n)$ are polynomials.

A distinguishing feature is the extremely good quality of the asymptotic approximations obtained; for instance 15 digits of accuracy is not uncommon in coefficients of index as low as 50.

IV. 4.1. Rational functions. A function f(z) is a *rational function* iff it is of the form $f(z) = \frac{N(z)}{D(z)}$, with N(z) and D(z) being polynomials, which me may always assume to be relatively prime. For rational functions that are generating functions, we have $D(0) \neq 0$.

Sequences $\{f_n\}_{n\geq 0}$ that are coefficients of rational functions coincide with sequences that satisfy linear recurrence relations with constant coefficients. To see it, compute $[z^n]f(z)$. D(z), with $n > \deg(N(z))$. If $D(z) = d_0 + d_1z + \cdots + d_mz^m$, then for n > m, one has:

$$\sum_{j=0}^{m} d_j f_{n-j} = 0.$$

The main theorem we prove here provides an *exact* finite expression for coefficients of f(z) in terms of the poles of f(z). Individual terms in corresponding expressions are sometimes called exponential polynomials.

THEOREM IV.6 (Expansion of rational functions). If f(z) is a rational function that is analytic at zero and has poles at points $\alpha_1, \alpha_2, \ldots, \alpha_m$, then there exist m polynomials $\{\Pi_j(x)\}_{j=1}^m$ such that:

(21)
$$f_n \equiv [z^n]f(z) = \sum_{j=1}^m \Pi_j(n)\alpha_j^{-n}$$

Furthermore the degree of Π_j is equal to the order of the pole of f at α_j minus one.

An expression of the form (21) is sometimes called an *exponential polynomial*.

PROOF. Since f(z) is rational it admits a partial fraction expansion. Thus, assuming without loss of generality that deg (D) > deg(N), we can decompose f into a finite sum

$$f(z) = \sum_{(\alpha,r)} \frac{c_{\alpha,r}}{(z-\alpha)^r},$$

where α ranges over the poles of f(z) and r is bounded from above by the multiplicity of α as a pole of f. Coefficient extraction in this expression results from Newton's expansion,

$$[z^{n}]\frac{1}{(z-\alpha)^{r}} = \frac{(-1)^{r}}{\alpha^{r}}[z^{n}]\frac{1}{(1-\frac{z}{\alpha})^{r}} = \frac{(-1)^{r}}{\alpha^{r}}\binom{n+r-1}{r-1}\alpha^{-n}$$

The binomial coefficient is a polynomial of degree r - 1 in n, and collecting terms associated with a given α yields the statement of the theorem.

Notice that the expansion (21) is also an asymptotic expansion in disguise: when grouping terms according to the α 's of increasing modulus, each group appears to be *exponentially smaller* than the previous one. A classical instance is the OGF of Fibonacci numbers,

$$f(z) = \frac{z}{1 - z - z^2} = \frac{z}{1 - z - z^2},$$

with poles at

$$\frac{-1+\sqrt{5}}{2} \doteq 0.61803, \qquad \frac{-1-\sqrt{5}}{2} \doteq -1.61803,$$

so that

$$F_n = \frac{1}{\sqrt{5}}\varphi^n - \frac{1}{\sqrt{5}}\bar{\varphi}^n = \frac{\varphi^n}{\sqrt{5}} + O(\frac{1}{\varphi^n}),$$

with $\varphi = (1 + \sqrt{5})/2$ the golden ratio, and $\bar{\varphi}$ its conjugate.

The next example is certainly an artificial one. It is simply designed to demonstrate that all the details of the full decomposition are usually not required. The rational function

$$f(z) = \frac{1}{(1-z^3)^2(1-z^2)^3(1-\frac{z^2}{2})}$$

has a pole of order 5 at z = 1, poles of order 2 at $z = \omega, \omega^2$ ($\omega = e^{2i\pi/3}$ a cubic root of unity), a pole of order 3 at z = -1, and simple poles at $z = \pm \sqrt{2}$. Therefore,

$$f_n = P_1(n) + P_2(n)\omega^{-n} + P_3(n)\omega^{-2n} + P_4(n)(-1)^n + P_5(n)2^{-n/2} + P_6(n)(-1)^n 2^{-n/2}$$

where the degrees of P_1, \ldots, P_6 are respectively 4, 1, 1, 2, 0, 0. For an asymptotic equivalent of f_n , only the pole at z = 1 needs to be considered since it corresponds to the fastest exponential growth; in addition, at z = 1, only the term of fastest growth needs to be taken into account since it gives the dominant contribution to coefficients. Thus, we have the correspondence

$$f(z) \sim \frac{1}{3^2 \cdot 2^3 \cdot (\frac{1}{2})} \frac{1}{(1-z)^5} \implies f_n \sim \frac{1}{3^2 \cdot 2^3 \cdot (\frac{1}{2})} \binom{n+4}{4} \sim \frac{n^4}{864}.$$

EXAMPLE 4. Asymptotics of denumerants. Denumerants are synonymous to integer partitions with summands restricted to be from a *fixed* finite set (Chapter I). We let $\mathcal{P}^{\mathcal{T}}$ be the class relative to set \mathcal{T} , with the known OGF,

$$P^{\mathcal{T}}(z) = \prod_{\omega \in \mathcal{T}} \frac{1}{1 - z^{\omega}}.$$

A particular case is the one of integer partitions whose summands are in $\{1, 2, ..., r\}$,

$$P^{\{1,\dots,r\}}(z) = \prod_{m=1}^{r} \frac{1}{1-z^m}$$

The GF has all its poles that are roots of unity. At z = 1, the order of the pole is r, and one has

$$P^{\{1,\dots,r\}}(z) \sim \frac{1}{r!} \frac{1}{(1-z)^r},$$

as $z \to 1$. Other poles have smaller multiplicity: for instance the multiplicity of z = -1 is equal to the number of factors $(1-z^{2j})^{-1}$ in $P^{\{1,\ldots,r\}}$, that is $\lfloor r/2 \rfloor$; in general a primitive *q*th root of unity is found to have multiplicity $\lfloor r/q \rfloor$. There results that z = 1 contributes a term of the form n^{r-1} to the coefficient of order *n*, while each of the other poles contributes a term of order at most $n^{\lfloor r/2 \rfloor}$. We thus find

$$P_n^{\{1,\dots,r\}} \sim c_r n^{r-1}$$
 with $c_r = \frac{1}{r!(r-1)!}$.

The same argument provides the asymptotic form of P_n^T , since, to first order asymptotics, only the pole at z = 1 counts. One then has:

PROPOSITION IV.2. Let T be a finite set of integers without a common divisor (gcd(T) = 1). The number of partitions with summands restricted to T satisfies

$$P_n^{\mathcal{T}} \sim \frac{1}{\tau} \frac{n^{r-1}}{(r-1)!}, \quad \text{with} \quad \tau := \prod_{n \in \mathcal{T}} n, \quad r := \operatorname{card}(\mathcal{T}).$$

For instance, in a country that would have pennies (1 cent), nickels (5 cents), dimes (10 cents) and quarters (25 cents), the number of ways to make change for a total of n cents is

$$[z^{n}]\frac{1}{(1-z)(1-z^{5})(1-z^{10})(1-z^{25})} \sim \frac{1}{1\cdot 5\cdot 10\cdot 25}\frac{n^{3}}{3!} \equiv \frac{n^{3}}{7500},$$

include:

asymptotically.

IV. 4.2. Meromorphic Functions. An expansion very similar to that of Theorem IV.6 given for rational functions holds true for the larger class of coefficients of meromorphic functions.

THEOREM IV.7 (Expansion of meromorphic functions). Let f(z) be a function meromorphic for $|z| \leq R$ with poles at points $\alpha_1, \alpha_2, \ldots, \alpha_m$, and analytic for |z| = R and z = 0. Then there exist m polynomials $\{\Pi_j(x)\}_{j=1}^m$ such that:

(22)
$$f_n \equiv [z^n] f(z) = \sum_{j=1}^m \Pi_j(n) \alpha_j^{-n} + \mathcal{O}(R^{-n}).$$

Furthermore the degree of Π_i is equal to the order of the pole of f at α_i minus one.

PROOF. We offer two different proofs, one based on subtracted singularities, the other one based on contour integration.

(i) Subtracted singularities. Around any pole α , f(z) can be expanded locally:

(23)
$$f(z) = \sum_{k \ge -M} c_{\alpha,k} (z - \alpha)^k$$

$$(24) \qquad \qquad = S_{\alpha}(z) + H_{\alpha}(z)$$

where the "singular part" $S_{\alpha}(z)$ is obtained by collecting all the terms with index in $[-M \dots -1] (S_{\alpha}(z) = N_{\alpha}(z)/(z-\alpha)^{M}$ with $N_{\alpha}(z)$ a polynomial of degree less than M) and $H_{\alpha}(z)$ is analytic at α . Thus setting $R(z) = \sum_{j} S_{\alpha_{j}}(z)$, we observe that f(z) - S(z) is analytic for $|z| \leq R$. In other words, by collecting the singular parts of the expansions and subtracting them, we have "removed" the singularities of f(z), whence the name of "method of subtracted singularities" sometimes given to the method [66, vol. 2, p. 448].

Taking coefficients, we get:

$$[z^{n}]f(z) = [z^{n}]S(z) + [z^{n}](f(z) - S(z)).$$

The coefficient of $[z^n]$ in the rational function S(z) is obtained from Theorem 1. It suffices to prove that the coefficient of z^n in f(z) - S(z), a function analytic for $|z| \leq R$, is $\mathcal{O}(R^{-n})$. This fact follows from trivial bounds applied to Cauchy's integral formula with the contour of integration being $\lambda = \{z \mid |z| = R\}$, as in the proof of Theorem IV.4:

$$|[z^{n}](f(z) - S(z))| = \frac{1}{2\pi} \left| \int_{|z|=R} (f(z) - S(z)) \frac{dz}{z^{n+1}} \right| \le \frac{1}{2\pi} \frac{\mathcal{O}(1)}{R^{n+1}} 2\pi R.$$

(ii) Contour integration. There is another line of proof for Theorem IV.7 which we briefly sketch as it provides an insight which is useful for applications to other types of singularities treated in Chapter V. It consists in using directly Cauchy's coefficient formula and "pushing" the contour of integration past singularities. In other words, one computes directly the integral

$$I_n = \frac{1}{2i\pi} \int_{|z|=R} f(z) \, \frac{dz}{z^{n+1}}$$

by residues. There is a pole at z = 0 with residue f_n and poles at the α_j with residues corresponding to the terms in the expansion stated in Theorem IV.7; for instance, if $f(z) \sim c/(z-a)$ as $z \to a$, then

$$\operatorname{Res}(f(z)z^{-n-1}, z=a) = \operatorname{Res}(\frac{c}{(z-a)}z^{-n-1}, z=a) = \frac{c}{a^{n+1}}.$$

Finally, by the same trivial bounds as before, I_n is $\mathcal{O}(R^{-n})$.

EXAMPLE 5. Surjections and alignments. The surjection EGF is $R(z) = (2 - e^z)^{-1}$, and we have already determined its poles: the one of smallest modulus is at $\log 2 \doteq 0.69314$.



FIGURE 8. The surjection numbers pyramid: for n = 2, 4, ..., 32, the exact values of the numbers R_n (left) compared to the approximation $\lceil \xi(n) \rceil$ with discrepant digits in boldface (right).

At the dominant pole, as z tends to $\log 2$, one has $R(z) \sim -\frac{1}{2}(z - \log 2)^{-1}$. This implies an approximation for the number of surjections:

$$R_n \equiv n! [z^n] R(z) \sim \xi(n),$$
 with $\xi(n) := \frac{n!}{2} \cdot \left(\frac{1}{\log 2}\right)^{n+1}.$

Here is, for n = 2, 4, ..., 32, a table of the values of the surjection numbers (left) compared with the asymptotic approximation rounded⁶ to the nearest integer, $\lceil \xi(n) \rfloor$: It is piquant to see that $\lceil \xi(n) \rfloor$ provides the exact value of R_n for all values of n = 1, ..., 15, and it starts losing one digit for n = 17, after which point a few "wrong" digits gradually appear, but in very limited number; see Figure 8 The explanation of such a faithful asymptotic representation owes to the fact that the error terms provided by meromorphic asymptotics are exponentially small. In effect, there is no other pole in $|z| \le 6$, the next ones being at $\log 2 \pm 2i\pi$ with modulus of about 6.32. Thus, for $r_n = [z^n]R(z)$, there holds

(25)
$$\frac{R_n}{n!} \sim \frac{1}{2} \cdot \left(\frac{1}{\log 2}\right)^{n+1} + \mathcal{O}(6^{-n}).$$

For the double surjection problem, $R^*(z) = (2 + z - e^z)$, we get similarly

$$[z^n]R^*(z) \sim \frac{1}{e^{\rho^*} - 1} \, (\rho^*)^{-n-1},$$

with $\rho^* = 1.14619$ the smallest positive root of $e^{\rho^*} - \rho^* = 2$. Alignments are sequences of cycles, with EGF

$$f(z) = \frac{1}{1 - \log(1 - z)^{-1}}$$

There is a singularity when $\log(1-z)^{-1} = 1$, which is at $z = 1 - e^{-1}$ and arises before z = 1 where the logarithm becomes singular. Thus the computation of the asymptotic form of f_n only needs a local expansion near $(1 - e^{-1})$:

$$f(z) \sim \frac{-e^{-1}}{z - 1 + e^{-1}} \implies [z^n]f(z) \sim \frac{e^{-1}}{(1 - e^{-1})^{n+1}}.$$

⁶The notation $\lceil x \rceil$ represents x rounded to the nearest integer: $\lceil x \rceil := \lfloor x + \frac{1}{2} \rfloor$.

▷ **21.** *Some "supernecklaces"*. One estimates

$$[z^n] \log\left(\frac{1}{1-\log\frac{1}{1-z}}\right) \sim \frac{1}{n}(1-e^{-1})^{-n},$$

where the EGF enumerates (labelled) cycles of cycles. [Hint: Take derivatives.]

EXAMPLE 6. *Generalized derangements.* The probability that the shortest cycle in a random permutation of size n has length larger than k is

$$[z^n] \frac{e^{-\frac{z}{1} - \frac{z^2}{2} - \dots - \frac{z^k}{k}}}{1 - z}.$$

For any fixed k, the generating function, call it f(z), is equivalent to $e^{-H_k}/(1-z)$ as $z \to 1$. Accordingly the coefficients $[z^n]f(z)$ tend to e^{-H_k} as $n \to \infty$. Thus, due to meromorphy, we have the characteristic implication

$$f(z) \sim \frac{e^{-H_k}}{1-z} \implies [z^n]f(z) \sim e^{-H_k}.$$

Since the difference between f(z) and the approximation at 1 is an entire function, the error is exponentially small:

(26)
$$[z^n] \frac{e^{-\frac{z}{1} - \frac{z^2}{2} - \dots - \frac{z^k}{k}}}{1 - z} = e^{-H_k} + O(R^{-n}),$$

for *fixed* k and *any* R > 1. The cases k = 1, 2 in particular justify the estimates mentioned in the introduction on p. 5.

As a side remark, the classical approximation of the harmonic numbers, $H_k \approx \log k + \gamma$ suggests $e^{-\gamma}/k$ as a further approximation to (26) that might be valid for both large n and large k in suitable regions. This can be made precise; in accordance with this heuristic argument, the expected length of the shortest cycle in a random permutation of size n is symptotic to

$$\sum_{k=1}^{n} \frac{e^{-\gamma}}{k} \sim e^{-\gamma} \log n$$

as first proved by Shepp and Lloyd in [101].

 \triangleright 22. Shortest cycles of permutations are not too long. Let S_n be the random variable denoting the length of the shortest cycle in a random permutation of size n. Using the circle |z| = 2 to estimate the error in the approximation e^{-H_k} above, one finds that, for $k \leq \log n$,

$$\left|\mathbb{P}(S_n > k) - e^{-H_k}\right| \le \frac{1}{2^n} e^{2^k},$$

which is exponentially small in this range of k-values. Thus, the approximation e^{-H_k} remains good when k is allowed to tend sufficiently slowly to ∞ with n. One can also explore the possibility of better bounds and larger regions of validity of the main approximation. (See Panario and Richmond's study [93] for a general theory of smallest components in sets.)

EXAMPLE 7. *Smirnov words and Carlitz compositions.* This examples illustrates the analysis of a group of rational generating functions (Smirnov words) paralleling nicely the enumeration of a special type of integer composition (Carlitz compositions) resorting to meromorphic asymptotics.

Bernoulli trials have been discussed in Chapter III, in relation to weighted word models. Take the class W of all words over an *r*-ary alphabet, where letter *j* is assigned

 \triangleleft

probability p_j and letters of words are drawn independently. With this weighting, the GF of all words is

$$W(z) = \frac{1}{1 - \sum p_j z} = \frac{1}{1 - z}.$$

Consider the problem of determining the probability that has a random word of length n is of Smirnov type, i.e., all blocks of length 2 are formed with two distinct letters (see also [**60**, p. 69]).

By our discussion of Section III.6, the GF of Smirnov words (again with the probabilistic weighting) is

$$S(z) = \frac{1}{1 - \sum \frac{p_j z}{1 + p_j z}}.$$

This is a rational function with a unique dominant singularity at ρ such that

(27)
$$\sum_{j=1}^{r} \frac{p_j \rho}{1 + p_j \rho} = 1.$$

(It is easy to verify by monotonicity that this equation has a unique positive solution.) Thus, ρ is a well characterized algebraic number defined implicitly by an equation of degree r. There results that the probability for a word to be Smirnov is (not too surprisingly) exponentially small, with the precise formula being

$$[z^n]S(z) \sim C \cdot \rho^{-n}, \qquad C = \left(\rho \sum \frac{p_i \rho}{1 + p_i \rho}\right)^{-1}$$

A similar analysis, but with bivariate generating functions shows that in a random word of length n conditioned to be Smirnov, the letter j appears with frequency asymptotic to

(28)
$$q_j = \frac{p_j \rho}{1 + p_j \rho},$$

in the sense that mean number of occurrences of letter j is asymptotic to $q_j n$. All these results are seen to be consistent with the equiprobable letter case $p_j = 1/r$, for which $\rho = r/(r-1)$.

Carlitz compositions illustrate a similar situation, in which the alphabet is in a sense infinite, while letters have different sizes. Recall that a Carlitz composition of the integer n is a composition of n such that no two adjacent summands have equal values. Consider first compositions with a bound m on the largest allowable summand. The OGF of such Carlitz compositions is

$$C^{[m]}(z) = \left(1 - \sum_{j=1}^{m} \frac{z^j}{1 + z^j}\right)^{-1},$$

and the OGF of all Carlitz compositions is obtained by letting m tend to infinity:

(29)
$$C^{[\infty]}(z) = \left(1 - \sum_{j=1}^{\infty} \frac{z^j}{1+z^j}\right)^{-1}$$

In particular, we get *EIS* **A003242**⁷:

$$C^{[\infty]}(z) = 1 + z + z^2 + 3z^3 + 4z^4 + 7z^5 + 14z^6 + 23z^7 + 39z^8 + 71z^9 + \cdots$$

⁷The *EIS* designates Sloane's On-Line Encyclopedia of Integer Sequences [102]; see [103] for an earlier printed version.



 $(1+1.02z^4)^{-3}(1-1.05z^5)^{-1}$ illustrate a periodic superposition of smooth behaviours that depend on the residue class of *n* modulo 20.

The asymptotic form of the number of Carlitz compositions is then easily found by singularity analysis of meromorphic functions. The OGF has a simple pole at ρ which is the smallest positive root of the equation

(30)
$$\sum_{j=1}^{\infty} \frac{\rho^j}{1+\rho^j} = 1.$$

(Note the formal analogy with (27) due to commonality of the combinatorial argument.)

 $C_n^{[\infty]} \sim C \cdot \alpha^n, \quad C \doteq 0.45638, \quad \alpha \doteq 1.75024.$

There, $\alpha = \rho$ with ρ as in (30). In a way analogous to Smirnov words, the asymptotic frequency of summand k appears to be $\rho^k/(1+\rho^k)$; see [71, 83] for further properties.

IV.5. Localization of singularities

There are situations where a function possesses several dominant singularities, that is, several singularities are present on the boundary of its disk of convergence. We examine here the induced effect on the coefficient's coefficients and discuss ways to localize such dominant singularities.

IV.5.1. Multiple singularities. In the presence of multiple singularities on the circle of convergence of a series, several geometric terms of the form α^n sharing the same modulus must be combined. In simpler cases, such terms induce a periodic behaviour for coefficients that is easy to describe; in the more general case, fluctuations of a somewhat "arithmetic nature" result. Finally, consideration of *all* singularities (whether dominant or not) of a meromorphic functions may lead to explicit summations expressing their coefficients.

Periodicities. When several singularities of f(z) have the same modulus, they may induce complete cancellations, so that different regimes will be present in the coefficients of f. For instance

$$\frac{1}{1+z^2} = 1 - z^2 + z^4 - z^6 + z^8 - \dots, \ \frac{1}{1-z^3} = 1 + z^3 + z^6 + z^9 + \dots,$$



FIGURE 10. The coefficients of $f = 1/(1 - \frac{6}{5}z + z^2)$ exhibit an apparently chaotic behaviour (left) which in fact corresponds to a discrete sampling of a sine function (right), reflecting the presence of two conjugate complex poles.

exhibit patterns of periods 4 and 3 respectively, this corresponding to roots of unity or order 4 $(\pm i)$, and 3. Accordingly,

$$\phi(z) = \frac{1}{1+z^2} + \frac{1}{1-z^3} = \frac{2-z^2+z^3+z^4+z^8+z^9-z^{10}}{1-z^{12}}$$

has a pattern of period 12, and the coefficients ϕ_n such that $n \equiv 1, 5, 6, 7, 11$ modulo 12 are zero. Consequently, if we analyze

$$[z^n]\psi(z)$$
 where $\psi(z) = \phi(z) + \frac{1}{1 - z/2}$,

we see that a different exponential growth manifests itself when n is taken congruent to $1, 5, 6, 7, 11 \mod 12$. In many combinatorial applications, generating functions involving periodicities can be decomposed "at sight", and the corresponding asymptotic subproblems generated are then solved separately.

▷ 23. Decidability of polynomial properties. Given a polynomial $p(z) \in \mathbb{Q}[z]$, the following properties are decidable: (i) whether one of the zeros of p is a root of unity; (ii) whether one of the zeros of p has an argument that is commensurate with π . [One can use resultants. An algorithmic discussion of this and related issues is given in [62].]

Nonperiodic fluctuations. Take the polynomial $D(z) = 1 - \frac{6}{5}z + z^2$, whose roots are

$$\alpha = \frac{3}{5} + i\frac{4}{5}, \ \bar{\alpha} = \frac{3}{5} - i\frac{4}{5},$$

both of modulus 1 (the numbers 3, 4, 5 form a Pythagorean triple), with argument $\pm \theta$ where $\theta = \arctan(\frac{4}{3}) = 0.9279$. The expansion of the function f(z) = 1/D(z) starts as

$$\frac{1}{1 - \frac{6}{5}z + z^2} = 1 + \frac{6}{5}z + \frac{11}{25}z^2 - \frac{84}{125}z^3 - \frac{779}{625}z^4 - \frac{2574}{3125}z^5 + \cdots$$

the sign sequence being

$$+++---++++---+++----++++----,$$

which indicates a mildly irregular oscillating behaviour, where blocks of 3 or 4 pluses follow blocks of 3 or 4 minuses.

The exact form of the coefficients of f results from a partial fraction expansion:

$$f(z) = \frac{a}{1 - z/\alpha} + \frac{b}{1 - z/\bar{\alpha}} \qquad \text{with } a = \frac{1}{2} + \frac{3}{8}i, \ b = \frac{1}{2} - \frac{3}{8}i.$$

Accordingly,

$$f_n = ae^{-in\theta_0} + be^{in\theta_0}$$
$$= \frac{\sin((n+1)\theta_0)}{\sin(\theta_0)}.$$

This explains the sign changes observed. Since the angle θ_0 is not commensurate with π , the coefficients fluctuate but, unlike in our earlier examples, no exact periodicity is present in the sign patterns. See Figure 10 for a rendering and Figure 10 below for a meromorphic case linked to compositions into prime summands.

Complicated problems of an arithmetical nature may occur if several such singularities with non–commensurable arguments combine, and some open problem remain in the analysis of linear recurring sequences. (For instance no decision procedure is known to determine whether such a sequence ever vanishes.) Fortunately, such problems occur infrequently in combinatorial enumerations where zeros of rational functions tend to have a simple geometry.

Exact formulæ. The error terms appearing in the asymptotic expansion of coefficients of meromorphic functions are already exponentially small. By "pealing off" the singularities of a meromorphic function layer by layer, in order of increasing modulus, one is led to extremely precise expansions for the coefficients. Sometimes even, "exact" expressions may result. The latter is the case for the Bernoulli numbers B_n , the surjection numbers R_n , the Secant numbers E_{2n} and the Tangent numbers E_{2n+1} defined by

$$\sum_{n=0}^{\infty} B_n \frac{z^n}{n!} = \frac{z}{e^z - 1} \quad \text{(Bernoulli numbers)}$$

$$\sum_{n=0}^{\infty} R_n \frac{z^n}{n!} = \frac{1}{2 - e^z} \quad \text{(Surjection numbers)}$$

$$\sum_{n=0}^{\infty} E_{2n} \frac{z^{2n}}{(2n)!} = \frac{1}{\cos(z)} \quad \text{(Secant numbers)}$$

$$\sum_{n=0}^{\infty} E_{2n+1} \frac{z^{2n+1}}{(2n+1)!} = \tan(z) \quad \text{(Tangent numbers)}.$$

Bernoulli numbers have an EGF $z/(e^z - 1)$ that has poles at the points $\chi_k = 2ik\pi$, with $k \in \mathbb{Z} \setminus \{0\}$. The residue at χ_k is equal to χ_k ,

$$\frac{z}{e^z - 1} \sim \frac{\chi_k}{z - \chi_k} \qquad (z \to \chi_k).$$

The expansion theorem for meromorphic functions is applicable here. To see it use the Cauchy integral formula, and proceed as in the proof of Theorem IV.7, using as external contours large circles that pass half way between poles. Along these contours, the integrand tends to 0 because the Cauchy "kernel" z^{-n-1} decreases with the radius of the integration contour while the EGF stays bounded. In the limit, corresponding to an infinitely large contour, the coefficient integral becomes equal to the sum of all residues of the meromorphic function over the whole of the complex plane.

From this argument, we thus get: $\frac{B_n}{n!} = -\sum_{k \in \mathbb{Z} \setminus \{0\}} \chi_k^{-n}$. This proves that $B_n = 0$ if *n* is odd. If *n* is even, then grouping terms two by two, we get the exact representation

(which also serves as an asymptotic expansion):

(31)
$$\frac{B_{2n}}{(2n)!} = (-1)^{n-1} 2^{1-2n} \pi^{-2n} \sum_{k=0}^{\infty} \frac{1}{k^{2n}}$$

Reverting the equality, we have also established that

$$\zeta(2n) = (-1)^{n-1} 2^{2n-1} \pi^{2n} \frac{B_{2n}}{(2n)!} \quad \text{with} \quad \zeta(s) = \sum_{k=1}^{\infty} \frac{1}{k^s}, \quad B_n = n! [z^n] \frac{z}{e^z - 1},$$

a well-known identity that provides values of the Riemann zeta function ($\zeta(s)$) at even integers as rational multiples of powers of π .

In the same vein, the *surjection numbers* have as EGF $R(z) = (2 - e^z)^{-1}$ with simple poles at

$$\chi_k = \log 2 + 2ik\pi$$
 where $R(z) \sim \frac{1}{2} \frac{1}{\chi_k - z}$.

Since R(z) stays bounded on circles passing half way in between poles, we find the exact formula, $\frac{R_n}{n!} = \frac{1}{2} \sum_{k \in \mathbb{Z}} \chi_k^{-n-1}$. An equivalent real formulation is

(32)
$$\frac{R_n}{n!} = \frac{1}{2} \left(\frac{1}{\log 2} \right)^{n+1} + \sum_{k=1}^{\infty} \frac{\cos((n+1)\theta_k)}{(\log^2 2 + 4k^2\pi^2)^{(n+1)/2}} \text{ with } \theta_k = \arctan(\frac{2k\pi}{\log 2}),$$

which shows the hidden occurrence of infinitely many "harmonics" of fast decaying amplitude.

 \triangleright 24. Alternating permutations, tangent and secant numbers. The relation (31) also provides a representation of the tangent numbers since $E_{2n-1} = (-1)^{n-1} B_{2n} 4^n (4^n - 1)/(2n)$. The secant numbers E_{2n} satisfy

$$\sum_{k=1}^{\infty} \frac{(-1)^k}{(2k+1)^{2n+1}} = \frac{(\pi/2)^{2n+1}}{2(2n)!} E_{2n},$$

which can be read either as providing an asymptotic expansion of E_{2n} or as an evaluation of the sums on the left (the values of a Dirichlet *L*-function) in terms of π . The asymptotic number of alternating permutations (Chapter II) is consequently known to great accuracy.

 \triangleright 25. Solutions to the equation $\tan(x) = x$. Let x_n be the *n*th positive root of the equation $\tan(x) = x$. For any integer $r \ge 1$, the sum $\sum_n x_n^{-2r}$ is a computable rational number. [From folklore and *The American Mathematical Monthly.*]

IV.5.2. Localization of zeros and poles. We gather here a few results that often prove useful in determining the location of zeros of analytic functions, and hence of poles of meromorphic functions. A detailed treatment of this topic may be found in Henrici's book [66].

Let f(z) be an analytic function in a region Ω and let γ be a simple closed curve interior to Ω , and on which f is assumed to have no zeros. We claim that the quantity

$$N(f;\gamma) = \frac{1}{2i\pi} \int_{\gamma} \frac{f'(z)}{f(z)} dz$$

exactly equals the number of zeros of f inside γ counted with multiplicity. The reason is that the function f'/f has its poles exactly at the zeros of f, and its residue at each pole is 1, so that the assertion directly results from the residue theorem

Since a primitive function of f'/f is $\log f$, the integral also represents the variation of $\log f$ along γ , which is written $[\log f]_{\gamma}$. The variation $[\log f]_{\gamma}$ reduces to *i* times the variation of the argument of *f* along γ as $\log(re^{i\theta}) = \log r + i\theta$ and the modulus *r* has



FIGURE 11. The transforms of $\gamma_j = \{|z| = \frac{4j}{10}\}$ by $P_4(z) = 1 - 2z + z^4$, for j = 1, 2, 3, 4, demonstrate that $P_4(z)$ has no zero inside |z| < 0.4, one zero inside |z| < 0.8, two zeros inside |z| < 1.2 and four zeros inside |z| < 1.6. The actual zeros are at $\rho_4 = 0.54368, 1$ and $1.11514 \pm 0.77184i$.

variation equal to 0 along a closed contour, $[\log \rho]_{\gamma} = 0$. The quantity $[\theta]_{\gamma}$ is, by its definition, the number of times the transformed contour $f(\gamma)$ winds about the origin. This observation is known as the *Argument Principle*:

Argument Principle. The number of zeros of f(z) (counted with multiplicities) inside γ equals the winding number of the transformed contour $f(\gamma)$ around the origin.

By the same argument, if f is meromorphic in $\Omega \ni \gamma$, then $N(f;\gamma)$ equals the difference between the number of zeros and the number of poles of f inside γ , multiplicities being taken into account. Figure 11 exemplifies the use of the argument principle in localizing zeros of a polynomial.

By similar devices, we get Rouché's theorem:

Rouché's theorem. Let the functions f(z) and g(z) be analytic in a region containing in its interior the closed simple curve γ . Assume that f and g satisfy |g(z)| < |f(z)| on the curve γ . Then f(z) and

$$f(z) + g(z)$$
 have the same number of zeros inside the interior domain delimited by γ .

The intuition behind Rouché's theorem is that, since |g| < |f|, then $f(\gamma)$ and $(f + g)(\gamma)$ must have the same winding number.

 \triangleright **26.** *Proof of Rouché's theorem.* Under the hypothesis of Rouché's theorem, for $0 \le t \le 1$ h(z) = (f(z) + tg(z)) is such that $N(h; \gamma)$ is both an integer and a continuous function of t in the given range. The conclusion of the theorem follows.

▷ 27. The fundamental theorem of algebra. Every complex polynomial p(z) of degree n has exactly n roots. A proof follows by Rouché's theorem from the fact that, for large enough |z| = R, the polynomial assumed to be monic is a "perturbation" of its leading term, z^n .

These principles form the basis of numerical algorithms for locating zeros of analytic functions. For instance, one can start from an initial domain and recursively subdivide it until roots have been isolated with enough precision—the number of roots in a subdomain being at each stage determined by numerical integration; see Figure 11 and refer for instance to [27] for a discussion. Such algorithms can even acquire the status of full proofs if one operates with guaranteed precision routines (using, e.g., careful implementations of interval arithmetics). Examples of use of the method will appear in the next sections.

 \triangleright **28.** *The analytic Implicit Function Theorem from residues.* The sum of the roots of the equation g(y) = 0 interior to γ equals

$$\frac{1}{2i\pi} \int_{\gamma} \frac{g'(y)}{g(y)} \, y \, dy.$$

Let F(z, y) be an analytic function in both z and y (i.e., it admits a convergent series expansion). If $F'_y(z_0, y_0) \neq 0$, then the function y(z) implicitly defined by F(z, y) = 0 and such that $y(z_0) = y_0$ is given by

$$y(z) = \frac{1}{2i\pi} \int_{\gamma} \frac{F'_y(z,y)}{F(z,y)} y \, dy$$

where γ is a small loop around y_0 . Deduce that y(z) is analytic at z_0 . (Note: this requires a modicum of analytic functions of two complex variables as is to be found, e.g., in [17].)

IV.5.3. The example of patterns in words. All patterns are not born equal. Surprisingly, in a random sequence of coin tossings, the pattern HTT is likely to occur much sooner (after 8 tosses on average) than the pattern HHH (needing 14 tosses on average); see the preliminary discussion in Chapter I. Questions of this sort are of obvious interest in the statistical analysis of genetic sequences. Say you discover that a sequence of length 100,000 on the four letters A, G, C, T contains the pattern *TACTAC* twice. Can this be assigned to chance or is this is likely to be a meaningful signal of some yet unknown structure? The difficulty here lies in quantifying precisely where the asymptotic regime starts, since, by Borges's Theorem (see the Note in Chapter I), sufficiently long texts will almost certainly contain any fixed pattern. The analysis of rational generating functions supplemented by Rouché's theorem provides definite answers to such questions.

We consider here the class \mathcal{W} of words over an alphabet \mathcal{A} of cardinality $m \geq 2$. A pattern \mathfrak{p} of some length k is given. As seen in Chapters I and III, its autocorrelation polynomial is central to enumeration. This polynomial is defined as $c(z) = \sum_{j=0}^{k-1} c_j z^j$, where c_j is 1 if \mathfrak{p} coincides with its kth shifted version and 0 otherwise. We consider here the enumeration of words containing the pattern \mathfrak{p} at least once, and dually of words excluding the pattern \mathfrak{p} . In other words, we look at problems like: What is the probability that a random of words of length n does (or does not) contain your name as a block of consecutive letters? The OGF of the class of words excluding p is, we recall,

(33)
$$S(z) = \frac{c(z)}{z^k + (1 - mz)c(z)}$$

and we shall start with the case m = 2 of a binary alphabet. The function S(z) is simply a rational function, but the location and nature of its poles is yet unknown. We only know *a priori* that it should have a pole in the positive interval somewhere between $\frac{1}{2}$ and 1 (by Pringsheim's Theorem and since its coefficients are in the interval $[1, 2^n]$, for *n* large enough). Here is a small list for patterns of length k = 3, 4 of the pole ρ nearest to the origin:

Length (k)	Types	c(z)	ρ
k = 3	aab, abb,	1	0.61803
	aba, bab	$1 + z^2$	0.56984
	aaa, bbb	$1 + z + z^2$	0.54368
k = 4	aaab, aabb, abbb,	1	0.54368
	aaba, abba, abaa,	$1 + z^{3}$	0.53568
	abab, baba	$1 + z^2$	0.53101
	aaaa, bbbb	$1 + z + z^2 + z^3$	0.51879

We thus expect ρ to be close to $\frac{1}{2}$ as soon as the pattern is long enough. In order to prove this, we are going to apply Rouché's Theorem to the denominator of (33).

As regards termwise domination of coefficients, the autocorrelation polynomials lies between 1 (for less correlated patterns like **aaa**...**b**) and $1 + z + \cdots + z^{k-1}$ (for the special case **aaa**...**a**). We set aside the special case of **p** having only equal letters, i.e., a "maximal" autocorrelation polynomial—this case is discussed at length in the next chapter. Thus, in this scenario, the autocorrelation polynomial starts as $1 + z^{\ell} + \cdots$ for some $\ell \ge 2$. Fix the number A = 0.6. On |z| = A, we have

(34)
$$|c(z)| \ge \left|1 - (A^2 + A^3 + \cdots)\right| = \left|1 - \frac{A^2}{1 - A}\right| = \frac{1}{10}$$

In addition, the quantity (1 - 2z) ranges over the circle of diameter [-0.2, 1.2] as z varies along |z| = A, so that $|1 - 2z| \ge 0.2$. All in all, we have found that, for |z| = A,

$$|(1-2z)c(z)| \ge 0.02.$$

On the other hand, for k > 7, we have $|z^k| < 0.017$ on the circle |z| = A. Then, amongst the two terms composing the denominator of (33), the first is strictly dominated by the second along |z| = A. By virtue of Rouché's Theorem, the number of roots of the denominator inside $|z| \le A$ is then same as the number of roots of (1-2z)c(z). The latter number is 1 (due to the root $\frac{1}{2}$) since c(z) cannot be 0 by the argument of (34). Figure 12 exemplifies the extremely well-behaved characters of the complex zeros.

In summary, we have found that for all patterns with at least two different letters $(\ell \ge 2)$ and length $k \ge 8$, the denominator has a unique root in $|z| \le A = 0.6$. The property for lengths k satisfying $4 \le k \le 7$ is then easily verified directly. The case $\ell = 1$ can be subjected to an entirely similar argument (see Chapter V for details). Therefore, unicity of a simple pole ρ of S(z) in the interval (0.5, 0.6) is granted.



FIGURE 12. Complex zeros of $z^{31} + (1-2z)c(z)$ represented as joined by a polygonal line: (left) correlated pattern $a(ba)^{15}$; (right) uncorrelated pattern $a(ab)^{15}$.

It is then a simple matter to determine the local expansion of s(z) near $z = \rho$,

$$S(z) \underset{z \to \rho}{\sim} \frac{\widetilde{\Lambda}}{\rho - z}, \qquad \widetilde{\Lambda} := \frac{c(\rho)}{2c(\rho) - k\rho^{k-1}},$$

from which a precise estimate for coefficients derives by Theorems IV.6 and IV.7.

The computation finally extends almost verbatim to nonbinary alphabets, with ρ being now close to $\frac{1}{m}$. It suffices to use the disc of radius A = 1.2/m. The Rouché part of the argument grants us unicity of the dominant pole in the interval (1/m, A) for $k \ge 5$ when m = 3, and for $k \ge 4$ and any $m \ge 4$. (The remaining cases are easily checked individually.)

PROPOSITION IV.3. Consider an m-ary alphabet. Let \mathfrak{p} be a pattern of length $k \ge 4$ with autocorrelation polynomial c(z). Then the probability that a random word of length n does not contain \mathfrak{p} as a pattern (a block of consecutive leters) satisfies

(35)
$$\mathbb{P}_{\mathcal{W}_n}(\mathfrak{p} \text{ does not occur}) = \Lambda_{\mathfrak{p}}(m\rho)^{-n-1} + O\left(\left(\frac{5}{6}\right)^n\right)$$

where $\rho \equiv \rho_p$ is the unique root in $(\frac{1}{m}, \frac{6}{5m})$ of the equation $z^k + (1 - mz)c(z) = 0$ and

$$\Lambda_{\mathfrak{p}} = \frac{mc(\rho)}{mc(\rho) - k\rho^{k-1}}.$$

Despite their austere appearance, these formulæ have indeed an a fairly intuitive content. First, the equation satisfied by ρ can be put under the form $mz = 1 + m^{-k}/c(z)$, and, since ρ is close to $\frac{1}{m}$, we may expect the approximation

$$m\rho \approx 1 + \frac{1}{\gamma m^k}$$

where $\gamma := c(m^{-1})$ satisfies $1 \le \gamma < m/(m-1)$. By similar principles, the probabilities in (35) should be approximately

$$\mathbb{P}_{\mathcal{W}_n}(\mathfrak{p} \text{ does not occur}) \approx \left(1 + \frac{1}{\gamma m^k}\right)^{-n} \approx e^{-n/(\gamma m^k)}.$$

For a binary alphabet, this tells us that the occurrence of a pattern of length k starts becoming likely when n is of the order of 2^k , that is, when k is of the order of $\log_2 n$. The more precise moment when this happens must depend (via γ) on the autocorrelation of the pattern, with strongly correlated patterns having a tendency to occur a little late. (This vastly generalizes our empirical observations of Chapter I.) However, observe that the mean number of occurrences of a pattern in a text of length n does not depend on the shape of the pattern. This apparent paradox is easily resolved: correlated patterns tend to occur late, but they lend themselves to appearing in clusters. Thus, the late pattern **aaa** when it occurs still has probability $\frac{1}{2}$ to occur at the next position as well, and cash in another occurrence, whereas no such possibility is available to the early pattern **aab** whose occurrences must be somewhat spread out.

Such analyses are important as they can be used to develop a precise understanding of the behaviour of data compression algorithms (the Lempel–Ziv scheme); see Julien Fayolle's memoir (Master Thesis, Paris, 2002) for details.

 \triangleright **29.** *Multiple pattern occurrences.* A similar analysis applies to the generating function $S^{(s)}(z)$ of words containing a fixed number s of occurrences of a pattern p. The OGF is obtained by expanding (with respect to u) the BGF W(z, u) obtained in Chapter III by means of an inclusion-exclusion argument. For $s \ge 1$, one finds

$$S^{\langle s \rangle}(z) = z^k \frac{N(z)^{s-1}}{D(z)^{s+1}}, \qquad D(z) = z^k + (1 - mz)c(z), \quad N(z) = z^k + (1 - mz)(c(z) - 1)),$$

 \triangleleft

which now has a pole of multiplicity s + 1 at $z = \rho$.

 \triangleright **30.** *Patterns in Bernoulli sequences.* Similar results hold when letters are assigned nonuniform probabilities, $p_j = \mathbb{P}(a_j)$, for $a_j \in \mathcal{A}$. One only needs to define the weighted autocorrelation polynomial by its coefficient c_j being $c_j = \mathbb{P}(\mathfrak{p}_1 \cdots \mathfrak{p}_j)$, when \mathfrak{p} coincides with its *j*th shifted version. Multiple pattern occurrences can be also analysed.

IV.6. Singularities and functional equations

In the various combinatorial examples discussed so far in this chapter, we have been dealing with functions that are given by explicit expressions. Such situations essentially cover nonrecursive structures as well as the simplest recursive structures, like Catalan or Motzkin trees, whose generating functions are expressible in terms of radicals. In fact, as will shall see extensively in this book, complex analytic methods are instrumental in analysing coefficients of functions *implicitly* specified by functional equations. In other words: *the very nature of a functional equation can often provide clues regarding the singularities of its solution*. Chapter V will illustrate this philosophy in the case of rational functions defined by systems of positive equations; a very large number of examples will then be given in Chapters VI and VII, where singularities much more general than mere poles are treated. The purpose of this subsection is simply to offer a preliminary discussion of the way dominant singularities can be located in many cases by means means of simple iteration or inversion properties of analytic functions. Three typical functional equations are to be discussed here:

$$f(z) = ze^{f(z)}, \qquad f(z) = z + f(z^2 + z^3), \qquad f(z) = \frac{1}{1 - zf(z^2)}.$$

Inverse functions. We start with a generic problem: given a function ψ analytic at a point y_0 with $z_0 = \psi(y_0)$ what can be said about its inverse, namely the solution(s) to the equation $\psi(y) = z$ when z is near z_0 and y near y_0 ? Two cases occur depending on the value of $\psi'(y_0)$.

Regular case. If $\psi'(y_0) \neq 0$, then ψ admits an analytic expansion near y_0 :

$$\psi(y) = \psi(y_0) + (y - y_0)\psi'(y_0) + \frac{1}{2}(y - y_0)^2\psi''(y_0) + \cdots$$

Solving formally for *y* indicates a *locally linear* dependency,

(36)
$$y - y_0 \sim \frac{1}{\psi'(y_0)}(z - z_0).$$

A full formal expansion of $y - y_0$ in powers of $z - z_0$ is obtained by repeated substitution,

(37)
$$y - y_0 = c_1(z - z_0) + c_2(z - z_0)^2 + \cdots$$

and the method of majorizing series shows that the series so obtained converges locally in a sufficiently small neighbourhood of z_0 . Rouché's theorem (equivalently, the analytic version of the Implicit Function Theorem, see Note 28), implies that the equation $\psi(y) = z$ admits there a unique analytic solution. In summary, an analytic function locally admits an analytic inverse near any point where its first derivative is nonzero.

Singular case. If to the contrary one has $\psi'(y_0) = 0$ and $\psi''(y_0) \neq 0$, then the expansion of ψ is of the form

(38)
$$\psi(y) = \psi(y_0) + \frac{1}{2}(y - y_0)^2 \psi''(y_0) + \cdots$$

Solving formally for y now indicates a *locally quadratic* dependency

$$(y-y_0)^2 \sim \frac{2}{\psi''(y_0)}(z-z_0),$$

and the inversion problem admits two solutions satisfying

$$y - y_0 \sim \pm \sqrt{\frac{2}{\psi''(y_0)}} (z - z_0)^{1/2}.$$

The point z_0 is thus a branch point.

A similar reasoning applies whenever the first nonzero derivative of ψ at y_0 is of order $r \ge 2$ (with a local behaviour for y then of the form $(z - z_0)^{1/r}$). Thus, the dependency between y and z cannot be analytic around (y_0, z_0) . In other words, an analytic function is not locally invertible in an analytic manner in the vicinity of any point where its first derivative is zero.

We can now consider the problem of obtaining information on the coefficients of a function y(z) defined by an implicit equation

(39)
$$y(z) = z\phi(y(z)).$$

For simplicity, we shall momentarily assume $\phi(u)$ to be a nonlinear entire function (possibly a polynomial of degree ≥ 2) with nonnegative coefficients. In order for the problem to be (formally) well-posed we assume that $\phi(0) \neq 0$.

The equation (39) occurs in the counting of various types of trees. For instance, $\phi(u) = e^u$ corresponds to labelled Cayley trees, $\phi(u) = (1 + u)^2$ to binary trees, and $\phi(u) = 1 + u + u^2$ to plane unary-binary trees (Motzkin trees). A full analysis of the problem was developed by Meir and Moon [85], themselves elaborating on earlier ideas of Pólya [97, 98] and Otter [92].

Equation (39) may be rephrased as

(40)
$$\psi(y(z)) = z$$
 where $\psi(u) = \frac{u}{\phi(u)}$,



FIGURE 13. Singularities of inverse functions: $\phi(u) = e^u$ (left); $\psi(u) = u/\phi(u)$ (middle); $y = \text{Inv}(\psi)$ (right).

so that it is a generic instance of the inversion problem for analytic functions: $y = \psi^{(-1)}$. We first observe that (39) and (40) admit unique formal power series solutions by the method of indeterminate coefficients. An application of the technique of majorizing series shows that this formal solution also represents an analytic function near the origin, with y(0) = 0. In addition, the coefficients of y(z) are all nonnegative.

Now comes the hunt for singularities. The function y(z) increases along the positive real axis. The equation $\psi'(\tau) = 0$ which is expected to create singularities for y(z) is in terms of ϕ :

(41)
$$\phi(\tau) - \tau \phi'(\tau) = 0.$$

The function $\phi(u) = \sum_{k=0}^{\infty} \phi_k u^k$ being by assumption entire, the equation (41) is equivalent to

$$\phi_0 = \phi_2 \tau^2 + 2\phi_3 \tau^3 + \cdots$$

which admits a unique positive solution.

As z increases, starting from 0 along the positive real axis, y(z) increases. Let $\rho \leq \infty$ be the dominant positive singularity of y(z). We are going to prove a contrario that $y(\rho) = \tau$ (technically, we should define $y(\rho)$ as the limit of y(x) as $x \to \rho^-$). Assume that $y(\rho) < \tau$; then y(z) could be analytically continued at $z = \rho$, by the discussion above of inverse functions in the regular case, since $\phi'(y(\rho)) > 0$. If on the other hand, we had $y(\rho) > \tau$, then, there would be a value $\rho^* < \rho$ such that $y(\rho^*) = \tau$; but there, we would have $\psi'(y(\rho^*)) = 0$, so that y(z) would be singular at $z = \rho^*$ by the discussion on inverse functions in the singular case. Thus, in both cases, the assumption $y(\rho) \neq \tau$ leads to a contradiction. We thus obtain that $y(\rho) = \tau$, and, since y and ψ are inverse functions, this corresponds to

$$\phi = \psi(\tau) = \tau/\phi(\tau).$$

Equipped with this discussion, we state a result which covers situations more general than the case of ϕ being entire.

PROPOSITION IV.4. Let ϕ be a nonlinear function that is analytic at 0, with nonnegative Taylor coefficients and radius of convergence $R \leq +\infty$. Assume that there exists $\tau \in (0, R)$ such that

(42)
$$\frac{\tau\phi'(\tau)}{\phi(\tau)} = 1$$

Let y(z) be the solution analytic at the origin of the equation $y(z) = \phi(y(z))$. Then, one has the exponential growth formula:

$$[z^n] y(z) \bowtie \left(\frac{1}{\rho}\right)^n$$
 where $\rho = \frac{\tau}{\phi(\tau)} = \frac{1}{\phi'(\tau)}$.

Note that, by Supplement 31 below, there can be *at most* one solution of the characteristic equation (42) in (0, R), a necessary and sufficient condition for the existence of a solution in the open interval (0, R) being $\lim_{x\to R^-} \frac{x\phi'(x)}{\phi(x)} > 1$. This last condition is automatically granted as soon as $\phi(R) = +\infty$.

PROOF. The discussion above applies verbatim. The function y(z) is analytic around 0 (by majorizing series techniques). By the already seen argument, its value $y(\rho)$ cannot be different from τ , so that its radius of convergence must equal ρ . The form of y_n then results from general exponential bounds.

 \triangleright **31.** Convexity of GFs and the Variance Lemma. Let $\phi(z)$ be a nonlinear GF with nonnegative coefficients and a nonzero radius of convergence R. For $x \in (0, R)$ a parameter, define the Boltzmann random variable Ξ (of parameter x) by the property

$$\mathbb{P}(\Xi = n) = \frac{\phi_n x^n}{\phi(x)}, \quad \text{with} \quad \mathbb{E}(s^{\Xi}) = \frac{\phi(sx)}{\phi(x)}$$

the probability generating function of Ξ . By differentiation, the first two moments of Ξ are

$$\mathbb{E}(\Xi) = \frac{x\phi'(x)}{\phi(x)}, \qquad \mathbb{E}(\Xi^2) = \frac{x^2\phi''(x)}{\phi(x)} + \frac{x\phi'(x)}{\phi(x)}.$$

0 44 5 5

There results, for any nonlinear GF $\phi(x)$, the general convexity inequality

$$\frac{d}{dx}\left(\frac{x\phi'(x)}{\phi(x)}\right) > 0$$

since the variance of a nondegenerate random variable is always positive. Equivalently, the function $\log(\phi(e^t))$ is convex for $t \in (-\infty, \log R)$.

Take for instance general Catalan trees corresponding to

$$y = \frac{z}{1 - y(z)}$$
, so that $\phi(u) = \frac{1}{1 - u}$.

We have R = 1 and the characteristic equation reads

$$\frac{\tau}{1-\tau} = 1$$

implying $\tau = \frac{1}{2}$, so that $\rho = \frac{1}{4}$. We obtain as anticipated $y_n \bowtie 4^n$, a weak asymptotic formula for the Catalan numbers. Similarly, for Cayley trees, we have $\phi(u) = e^u$, the characteristic equation reduces to $(\tau - 1)e^{\tau} = 0$, so that $\tau = 1$ and $\rho = e^{-1}$, giving a weak form of Stirling's formula:

$$[z^n]y(z) = \frac{n^{n-1}}{n!} \bowtie e^n.$$

Here is a table of a few cases of application of the method to structures already encountered in previous chapters.

Туре	$\phi(u)$	(R)	au, ho	$y_n \bowtie \rho^{-n}$
gen. Catalan tree	$\frac{1}{1-u}$	(1)	$\frac{1}{2}, \frac{1}{4}$	$y_n \bowtie 4^n$
binary tree	$(1+u)^2$	(∞)	$1, \frac{1}{4}$	$y_n \bowtie 4^n$
Motzkin tree	$1 + u + u^2$	(∞)	$1, \frac{1}{3}$	$y_n \bowtie 3^n$
Cayley tree	e^u	(∞)	$1,e^{-1}$	$y_n \bowtie e^n$

In fact, for all such problems, the dominant singularity is always of the square-root type as our previous discussion suggests. Accordingly, the asymptotic form of coefficients is invariably of the type

$$[z^n] y(z) \sim C \cdot \rho^{-n} n^{-3/2}$$

as we shall prove in Chapter VI by means of the singularity analysis method.

▷ **32.** A variant form of the inversion problem. Consider the equation $y = z + \phi(y)$, where ϕ is assumed to be entire and $\phi(u) = O(u^2)$ at u = 0. This corresponds to a simple variety of trees in which trees are counted by the number of their leaves only. For instance, we have already encountered labelled hierarchies (phylogenetic trees) in Section II.6 corresponding to $\phi(u) = e^u - 1 - u$, which is one of "Schröder's problems". Let $\tilde{\tau}$ be the root of $\phi'(\tilde{\tau}) = 1$ and set $\tilde{\rho} = \tilde{\tau} - \phi(\tilde{\tau})$. Then $[z^n]y(z) \bowtie \rho^{-n}$. For the EGF *L* of labelled hierarchies ($L = z + e^L - 1 - L$), this gives $L_n/n! \bowtie (2\log 2 - 1)^{-n}$. (Observe that Lagrange inversion also provides $[z^n]y(z) = \frac{1}{n}[w^{n-1}](1 - y^{-1}\phi(y))^{-n}$.)

Iteration. Consider the class \mathcal{E} of *balanced 2–3 trees* defined as trees whose node degrees are restricted to the set $\{0, 2, 3\}$, with the additional property that all leaves are at the same distance from the root. Such tree trees, which are particular cases of *B*-trees, are a useful data structure for implementing dynamic dictionaries [75]. We adopt as notion of size the number of leaves (also called external nodes). The OGF of \mathcal{E} satisfies the functional equation

(43)
$$E(z) = z + E(z^2 + z^3),$$

which reflects an inductive definition involving a substitution: given an existing tree, a new tree is obtained by substituting in all possible ways to each external node (\Box) either a pair (\Box, \Box) or a triple (\Box, \Box, \Box) . On other words, we have

$$\mathcal{E}[\Box] = \Box + \mathcal{E}\bigg[\Box \to (\Box\Box + \Box\Box\Box)\bigg].$$

Equation (43) implies the seemingly innocuous recurrence

$$E_n = \sum_{k=0}^n \binom{k}{n-2k} E_k$$
 with $E_0 = 0, E_1 = 1,$

but no closed-form solution is known (nor likely to exist) for E_n or E(z). The expansion starts as (the coefficients are *EIS* A014535)

$$E(z) = z + z^{2} + z^{3} + z^{4} + 2z^{5} + 2z^{6} + 3z^{7} + 4z^{8} + 5z^{9} + 8z^{10} + \cdots$$

We present here the first stage of an analysis due to Odlyzko [88] and corresponding to exponential bounds. Let $\sigma(z) = z^2 + z^3$. Equation (43) can be expanded by iteration in the ring of formal power series,

(44)
$$E(z) = z + \sigma(z) + \sigma^{[2]}(z) + \sigma^{[3]}(z) + \cdots,$$



FIGURE 14. The iterates of a point $x_0 \in [0, \frac{1}{\varphi}]$ (here $x_0 = 0.6$) by $\sigma(z) = z^2 + z^3$ converge fast to 0.

where $\sigma^{[j]}(z)$ denotes the *j*th iterate of the polynomial σ :

$$\sigma^{[0]}(z) = z, \qquad \sigma^{[h+1]}(z) = \sigma^{[h]}(\sigma(z)) = \sigma(\sigma^{[h]}(z)).$$

Thus, E(z) is nothing but the sum of all iterates of σ . The problem is to determine the radius of convergence of E(z), and by Pringsheim's theorem, the quest for dominant singularities can be limited to the positive real line.

For z > 0, the polynomial $\sigma(z)$ has a unique fixed point, $\rho = \sigma(\rho)$, at

$$ho = rac{1}{arphi} \qquad ext{where} \qquad arphi = rac{1+\sqrt{5}}{2},$$

the golden ratio. Also, for any positive x satisfying $x < \rho$, the iterates $\sigma^{[j]}(x)$ must converge to 0; see Fig. 14. Furthermore, since $\sigma(z) \sim z^2$ near 0, these iterates converge to 0 doubly exponentially fast. First, for $x \in [0, \frac{1}{2}]$, one has $\sigma(x) \leq \frac{3}{2}x^2$ for $x \in [0, \frac{1}{2}]$, so that there

(45)
$$\sigma^{[j]}(x) \le \left(\frac{3}{2}\right)^{2^{j}-1} x^{2^{j}}$$

Second, for $x \in [0, A]$, where A is any number $< \rho$, there is a number k_A such that $\sigma^{[k_A]}(x) < \frac{1}{2}$, so that, by (45), there holds:

$$\sigma^{[k]}(x) \le \frac{3}{2} \left(\frac{3}{4}\right)^{2^{k-k_A}}$$

Thus, the series of iterates of σ is quadratically convergent for $z \in [0, A]$, any $A < \rho$.

By the triangular inequality, $|\sigma(z)| \leq (\sigma(|z|))$, the sum in (44) is a normally converging sum of analytic functions, and is thus itself analytic. Consequently E(z) is analytic in the whole of the open disk $|z| < \rho$.



FIGURE 15. Left: the fractal domain of analyticity of E(z) in gray with darker areas representing faster convergence of the sum of iterates of σ . Right: the ratio $E_n/(\varphi^n n^{-1})$ plotted against $\log n$ for n = 1..500 confirms that $E_n \bowtie \varphi^n$ and illustrates the periodic fluctuations expressed by Equation (47).

It remains to prove that the radius of convergence of E(z) is exactly equal to ρ . To that purpose it suffices to observe that E(z), as given by (44), satisfies

$$E(x) \to +\infty$$
 as $x \to \rho^-$.

Let N be an arbitrarily large but fixed integer. It is possible to select a positive x_N sufficiently close to ρ with $x_N < \rho$, such that the Nth iterate $\sigma^{[N]}(x_N)$ is larger than $\frac{1}{2}$ (the function $\sigma^{[N]}(x)$ admits ρ as a fixed point and it is continuous and increasing at ρ). Given the sum expression (44), this entails the lower bound $E(x_N) > \frac{N}{2}$ for such an $x_N < \rho$ so that E(x) is unbounded as $x \to \rho^-$.

The dominant positive real singularity of E(z) is thus $\rho = \frac{1}{\varphi}$, and application of Cauchy bounds shows that

(46)
$$[z^n] E(z) \bowtie \left(\frac{1+\sqrt{5}}{2}\right)^n.$$

It is notable that this estimate could be established so simply by a purely qualitative examination of the basic functional equation and of a fixed point of the associated iteration scheme.

The complete asymptotic analysis of the E_n was given by Odlyzko [88] in a classic paper. It requires the full power of singularity analysis methods to be developed in Chapter VI. Equation (47) below states the end result, which involves periodic fluctuations; see Figure 15 (right). There is overconvergence of the representation (44), that is, convergence in certain directions beyond the disc of convergence of E(z), as illustrated by Figure 15 (left). The proof techniques involve an investigation of the behaviour of iterates of σ in the complex plane, an area launched by Fatou and Julia in the first half of the past century and nowadays well-studied under the name of "complex dynamics".

> 33. *The asymptotic number of 2–3 trees.* This analysis is from [88, 89]. The number of 2–tree trees satisfies asymptotically

(47)
$$E_n = \frac{\varphi^n}{n} \Omega(\log n) + O\left(\frac{\varphi^n}{n^2}\right),$$

where Ω is a periodic function with mean value $\varphi(\log(4-\varphi) \doteq 0.71208)$ and period $\log(4-\varphi) \doteq$. Thus oscillations are inherent in E_n . A plot of the ratio $E_n/(\phi^n/n)$ is offered in Figure 15. **Complete asymptotics of a functional equation.** This is Pólya's counting of certain molecules, a case where only a functional equation is known for a generating function, $M(z) = \sum_{n} M_{n} z^{n}$:

(48)
$$M(z) = \frac{1}{1 - zM(z^2)}$$

The M_n represent the number of chemical isomeres of alcohols $C_n H_{2n+1}OH$ without asymmetric carbon atoms, and the series starts as (*EIS* A000621)

(49)
$$M(z) = 1 + z + z^2 + 2z^3 + 3z^4 + 5z^5 + 8z^6 + 14z^7 + 23z^8 + 39z^9 + \cdots$$

By iteration of the functional equation, one finds a continued fraction representation:

$$M(z) = \frac{1}{1 - \frac{z}{1 - \frac{z^2}{1 - \frac{z^4}{\cdot}}}}.$$

Pólya [98] who established this functional equation in the historical paper that introduced "Pólya Theory" developed at the same time a precise asymptotic estimate for M_n .

PROPOSITION IV.5. Let M(z) be the solution analytic around 0 of the functional equation

$$M(z) = \frac{1}{1 - zM(z^2)}.$$

Then, there exist constants K and α such that

 $M_n \sim K \cdot \alpha^n$, $\alpha \doteq 1.6813675244$, $K \doteq 0.3607140971$.

PROOF. We offer two proofs. The first one is based on direct consideration of the functional equation and is of a high degree of applicability. The second one, following Pólya, makes explicit a linear structure present in the problem and leads to more explicit results.

First proof. The first few coefficients of M are determined by the functional equation and known (49). Then, by positivity of the functional equation, M(z) dominates coefficientwise any GF $(1 - zM_{< m}(z^2)^{-1})$, where $M_{< m}(z)$ is the *m*th truncation of M(z). In particular, one has the domination relation (use $M_{< 2}(z) = 1 + z$)

$$M(z) \preceq \frac{1}{1 - z - z^3}.$$

Since the rational fraction has a dominant poles at $z \doteq 0.68232$, this implies that the radius ρ of convergence of M(z) satisfies $\rho < 0.69 < 1$. In the other direction, since $M(z^2) < M(z)$ for $z \in (0, \rho)$, then, one has the numerical inequality

$$M(z) \le \frac{1}{1 - zM(z)}, \qquad 0 \le z < \rho.$$

This can be used to show that the Catalan generating function $C(z) = (1 - \sqrt{1 - 4z})/(2z)$ is a majorant of M(z) on the interval $(0, \frac{1}{4})$ and that M(z) exists for $z \in (0, \frac{1}{4})$. In other words, one has $\frac{1}{4} \leq \rho < 0.69$. At any rate, the radius of convergence of M is strictly between 0 and 1.

▷ **34.** Alcohols and trees. Since M(z) starts as $1+z+z^2+\cdots$ while C(z) starts as $1+z+2z^2+\cdots$, there is a small interval $(0, \epsilon)$ such that $M(z) \leq C(z)$. By the functional equation of M(z), one has $M(z) \leq C(z)$ for z in the larger interval $(0, \sqrt{\epsilon})$. One can then bootstrap and show that $M(z) \leq C(z)$ for $z \in (0, \frac{1}{4})$.

Next, as $z \to \rho^-$, one must have $zM(z^2) \to 1$. Indeed, if this was not the case, we would have $zM(z^2) < A < 1$ for some A. But then, since $\rho^2 < \rho$, the quantity $(1 - zM(z^2))^{-1}$ would be analytic at $z = \rho$, a clear contradiction. Thus, ρ is determined implicitly by the equation

$$\rho M(\rho^2) = 1,$$

and by monotonicity, there can be only one such solution. Numerically, one can estimate ρ as the limit of quantities ρ_m satisfying

$$\sum_{n=0}^{m} M_n \rho_m^{2n+1} = 1,$$

together with $\rho \in [\frac{1}{4}, 0.069]$. In each case, only a few of the M_n are needed. One obtains in this way:

$$\rho_{10} \doteq 0.595, \ \rho_{20} \doteq 0.594756, \ \rho_{30} \doteq 0.59475397, \ \rho_{40} \doteq 0.594753964,$$

and it is not hard to verify that this provides a geometrically convergent scheme to the limit $\rho \doteq 0.59475\,39639$. (Note: Pólya determined ρ to five decimals by hand!)

The previous discussion also implies that ρ is a pole, which must be simple. Thus

(50)
$$M(z) \sim z \to \rho K \frac{1}{1 - z/\rho}, \qquad K := \frac{1}{\rho M(\rho^2) + 2\rho^3 M'(\rho^2)}$$

The argument shows at the same time that M(z) is meromorphic in $|z| < \sqrt{\rho} \doteq 0.77$. That M(z) is a the only pole on $|z| = \rho$ can be seen from the fact that $zM(z^2) = z + z^3 + \cdots$ is unperiodic in the sense of Chapter V. (We don't detail the argument here as the property is also implied by the developments of the second proof.) The translation of the singular expansion (50) yields the statement.

Second proof. First, a sequence of formal approximants follows from (48) starting with

$$1, \ \frac{1}{1-z}, \ \frac{1}{1-\frac{z}{1-z^2}} = \frac{1-z^2}{1-z-z^2}, \ \frac{1}{1-\frac{z}{1-\frac{z^2}{1-z^4}}} = \frac{1-z^2-z^4}{1-z-z^2-z^4+z^5}.$$

which permits to compute any number of terms of the series M(z). Closer examination of (48) suggests to set

$$M(z) = \frac{\psi(z^2)}{\psi(z)},$$

where

$$\psi(z) = 1 - z - z^2 - z^4 + z^5 - z^8 + z^9 + z^{10} + z^{17} + z^{18} + z^{20} - z^{21} - z^{37} - \cdots$$

Back substitution into (48) yields

$$\frac{\psi(z^2)}{\psi(z)} = \frac{1}{1 - z\frac{\psi(z^4)}{\psi(z^2)}} \text{ or } \frac{\psi(z^2)}{\psi(z)} = \frac{\psi(z^2)}{\psi(z^2) - z\psi(z^4)},$$

which shows $\psi(z)$ to be a solution of the functional equation

$$\psi(z) = \psi(z^2) - z\psi(z^4).$$

The coefficients of ψ are all in the set $\{0, -1, +1\}$, as they satisfy the recurrence

$$\psi_{4n} = \psi_{2n}, \ \psi_{4n+1} = -\psi_n, \ \psi_{4n+2} = \psi_{2n+1}, \ \psi_{4n+3} = 0.$$

Thus, M(z) appears as the quotient of two function, $\psi(z^2)/\psi(z)$; since $\psi(z)$ whose coefficients are bounded by 1 in absolute value, it is analytic in the unit disk, M(z) is itself meromorphic in the unit disc. A numerical plot shows that that $\psi(z)$ has its smallest positive real zero at $\rho \doteq 0.59475$, which is a simple zero of $\psi(z)$ and thus a pole of M(z) as $\psi(\rho^2) \neq 0$. Thus

$$M(z) \sim \frac{\psi(\rho^2)}{(z-\rho)\psi'(\rho)} \implies M_n \sim -\frac{\psi(\rho^2)}{\rho\psi'(\rho)} \left(\frac{1}{\rho}\right)^n.$$

Numerical computations then yield Pólya's estimate. Et voilà!

The example of Pólya's alcohols is exemplary, both from a historical point of view and from a methodological perspective. It demonstrates that quite a lot of information can be pulled out of a functional equation without solving it. (A very similar situation will be discussed in Chapter V, see the enumeration of coin fountains.) In passing, we have made great use of the fact that if f(z) is analytic in |z| < r and some bounds imply the strict inequalities 0 < r < 1, then one can regard functions like $f(z^2)$, $f(z^3)$, and so on, as "known" since they are analytic in the disc of convergence of f and even beyond, a situation evocative of our earlier discussion of Pólya operators in Subsection IV. 3.3. Globally, the lesson is that functional equation, even very complicated ones, can often be used to bootstrap the local singular behaviour of solutions and one can do so despite the absence of any explicit solution. Then, the transition from singularities to coefficient asymptotics is a simple jump.

 \triangleright **35.** An arithmetic exercise Find a characterization of $\psi_n = [z^n]\psi(z)$ based on the binary representation of n. Tabulate ψ_n for all $n \in (10^{1000}, 10^{1000} + 10^{500})$, possibly using some compressed format. Find the asymptotic proportion of the ψ_n for $n \in [1..N]$ that are nonzero.

IV.7. Notes

This chapter has been designed to serve as a refresher of basic complex analysis, with special emphasis on methods relevant for analytic combinatorics. References most useful for the discussion given in this chapter include the books of Titchmarsh [109] (oriented towards classical analysis), Whittaker and Watson [114] (stressing special functions), Dieudonné [28] and Knopp [72]. Henrici [66] presents complex analysis under the perspective of constructive and numerical methods, a highly valuable point of view for this book. References dealing specifically with asymptotic analysis are discussed at the end of the next chapter.

As demonstrated by the first batch of examples sprinkled over this chapter, singularities provide a royal road to coefficient asymptotics. In this regard, the two main statements of this chapter are are the theorems relative to the expansion of rational and meromorphic functions, Theorems IV.6 and IV.7. They are of course extremely classical (and easy) results. Issai Schur (1875–1941) is to be counted amongst the very first mathematicians who recognized the rôle of analytic methods in combinatorial enumerations (Example 4). This thread was developed by George Pólya in his famous paper of 1937 (see [**97**, **98**]), which Read in [**98**, p. 96] describes as a "landmark in the history of combinatorial analysis". There, Pólya founded at the same time combinatorial chemistry, the enumeration of objects under group actions, and the complex-asymptotic theory of graphs and trees. De Bruijn's classic booklet [25] is a wonderfully concrete introduction to effective asymptotic theory, and it contains many examples from discrete mathematics thoroughly worked out. The state of affairs in 1995 regarding analytic methods in combinatorial enumeration is superbly summarized in Odlyzko's scholarly chapter [89]. Wilf devotes his Chapter 5 of *Generatingfunctionoloy* [116] to this question. The books by Hofri [68] and Szpankowski [108] contain useful accounts in the perspective of analysis of algorithms. See also our book [100] for a light introduction and the chapter by Vitter and Flajolet [112] for more on this topic.

Paraphrasing the number theorist Hecke, we may feel confident in stating: A function's singularities contain a wealth of asymptotic information on the function's coefficients; a generating function contains a wealth of information on the corresponding combinatorial structures. This philosophy furthermore unites analytic combinatorics and analytic number theory. It is the purpose of the next four chapters to illustrate it thoroughly by means of a great variety of combinatorial examples.

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