Analytic Combinatorics

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ANALYTIC COMBINATORICS

Analytic combinatorics aims to enable precise quantitative predictions of the properties of large combinatorial structures. The theory has emerged over recent decades as essential both for the analysis of algorithms and for the study of scientific models in many disciplines, including probability theory, statistical physics, computational biology and information theory. With a careful combination of symbolic enumeration methods and complex analysis, drawing heavily on generating functions, results of sweeping generality emerge that can be applied in particular to fundamental structures such as permutations, sequences, strings, walks, paths, trees, graphs and maps.

This account is the definitive treatment of the topic. In order to make it self-contained, the authors give full coverage of the underlying mathematics and give a thorough treatment of both classical and modern applications of the theory. The text is complemented with exercises, examples, appendices and notes throughout the book to aid understanding. The book can be used as a reference for researchers, as a textbook for an advanced undergraduate or a graduate course on the subject, or for self-study.

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Preface

ANALYTIC COMBINATORICS aims at predicting precisely the properties of large structured combinatorial configurations, through an approach based extensively on analytic methods. Generating functions are the central objects of study of the theory.

Analytic combinatorics starts from an exact enumerative description of combinatorial structures by means of generating functions: these 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. Singularities determine a function's coefficients in asymptotic form and lead to precise estimates for counting sequences. This chain of reasoning applies to a large number of problems of discrete mathematics relative to words, compositions, partitions, trees, permutations, graphs, mappings, planar configurations, and so on. A suitable adaptation of the methods also opens the way to the quantitative analysis of characteristic parameters of large random structures, via a perturbational approach.

THE APPROACH to quantitative problems of discrete mathematics provided by analytic combinatorics can be viewed as an *operational calculus* for combinatorics organized around three components.

> *Symbolic methods* develops systematic relations between some of the major constructions of discrete mathematics and operations on generating functions that exactly encode counting sequences.
> *Complex asymptotics* elaborates a collection of methods by which one can extract asymptotic counting information from generating functions, once these are viewed as analytic transformations of the complex domain. Singularities then appear to be a key determinant of asymptotic behaviour.
> *Random structures* 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, these questions are treated by a deformation (adding auxiliary variables) and a perturbation (examining the effect of small variations of such auxiliary variables) of the standard enumerative theory.

The present book expounds this view by means of a very large number of examples concerning classical objects of discrete mathematics and combinatorics. The eventual goal is an effective way of quantifying metric properties of large random structures.

Given its capacity of quantifying properties of large discrete structures, *Analytic Combinatorics* is susceptible to many applications, not only within combinatorics itself, but, perhaps more importantly, within other areas of science where discrete probabilistic models recurrently surface, like statistical physics, computational biology, electrical engineering, and information theory. Last but not least, the analysis of algorithms and data structures in computer science has served and still serves as an important incentive for the development of the theory.

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Part A: Symbolic methods. This part specifically develops *Symbolic methods*, which constitute a unified algebraic theory dedicated to setting up functional relations between counting generating functions. As it turns out, a collection of general (and simple) theorems provide a systematic translation mechanism between combinatorial constructions and operations on generating functions. This translation process is a purely formal one. In fact, with regard to basic counting, two parallel frameworks coexist—one for unlabelled structures and ordinary generating functions, the other for labelled structures and exponential generating functions. Furthermore, within the theory, parameters of combinatorial configurations can be easily taken into account by adding supplementary variables. Three chapters then form Part A: Chapter I deals with unlabelled objects; Chapter II develops labelled objects in a parallel way; Chapter III treats multivariate aspects of the theory suitable for the analysis of parameters of combinatorial structures.

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Part B: Complex asymptotics. This part specifically expounds *Complex asymptotics*, which is a unified analytic theory dedicated to the process of extracting asymptotic information from counting generating functions. A collection of general (and simple) theorems now provide a systematic translation mechanism between generating functions and asymptotic forms of coefficients. Five chapters form this part. Chapter IV serves as an *introduction to complex-analytic methods* and proceeds with the treatment of *meromorphic functions*, that is, functions whose singularities are poles, *rational functions* being the simplest case. Chapter V develops *applications of rational and meromorphic asymptotics of generating functions*, with numerous applications related to words and languages, walks and graphs, as well as permutations. Chapter VI develops a general theory of *singularity analysis* that applies to a wide variety of singularity types, such as square-root or logarithmic, and has consequences regarding trees as well as other recursively-defined combinatorial classes. Chapter VII presents *applications of singularity analysis* to 2–regular graphs and polynomials, trees of various sorts, mappings, context-free languages, walks, and maps. It contains in particular a discussion of the analysis of coefficients of algebraic functions. Chapter VIII explores *saddle-point methods*, which are instrumental in analysing functions with a violent growth at a singularity, as well as many functions with a singularity only at infinity (i.e., entire functions).

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Part C: Random structures. This part is comprised of Chapter IX, which is dedicated to the analysis of multivariate generating functions viewed as deformation and perturbation of simple (univariate) functions. Many known laws of probability theory, either discrete or continuous, from Poisson to Gaussian and stable distributions, are found to arise in combinatorics, by a process combining symbolic methods, complex asymptotics, and perturbation methods. As a consequence, many important characteristics of classical combinatorial structures can be precisely quantified in distribution.

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Part D: Appendices. Appendix A summarizes some key elementary concepts of combinatorics and asymptotics, with entries relative to asymptotic expansions, languages, and trees, among others. Appendix B recapitulates the necessary background in complex analysis. It may be viewed as a self-contained minicourse on the subject, with entries relative to analytic functions, the Gamma function, the implicit function theorem, and Mellin transforms. Appendix C recalls some of the basic notions of probability theory that are useful in analytic combinatorics.

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THIS BOOK is meant to be reader-friendly. Each major method is abundantly illustrated by means of concrete *Examples*[1] treated in detail—there are scores of them, spanning from a fraction of a page to several pages—offering a complete treatment of a specific problem. These are borrowed not only from combinatorics itself but also from neighbouring areas of science. With a view to addressing not only mathematicians of varied profiles but also scientists of other disciplines, *Analytic Combinatorics* is self-contained, including ample appendices that recapitulate the necessary background in combinatorics, complex function theory, and probability. A rich set of short *Notes*—there are more than 450 of them—are inserted in the text[2] and can provide exercises meant for self-study or for student practice, as well as introductions to the vast body of literature that is available. We have also made every effort to focus on *core ideas* rather than technical details, supposing a certain amount of mathematical maturity but only basic prerequisites on the part of our gentle readers. The book is also meant to be strongly problem-oriented, and indeed it can be regarded as a manual, or even a huge algorithm, guiding the reader to the solution of a very large variety of problems regarding discrete mathematical models of varied origins. In this spirit, many of our developments connect nicely with computer algebra and symbolic manipulation systems.

COURSES can be (and indeed have been) based on the book in various ways. Chapters I–III on *Symbolic methods* serve as a systematic yet accessible introduction to the formal side of combinatorial enumeration. As such it organizes transparently some of the rich material found in treatises[3] such as those of Bergeron–Labelle–Leroux, Comtet, Goulden–Jackson, and Stanley. Chapters IV–VIII relative to *Complex asymptotics* provide a large set of concrete examples illustrating the power

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[1] Examples are marked by "*Example* ⋯ ■".

[2] Notes are indicated by ▷ ⋯ ◁.

[3] References are to be found in the bibliography section at the end of the book.

of classical complex analysis and of asymptotic analysis outside of their traditional range of applications. This material can thus be used in courses of either pure or applied mathematics, providing a wealth of non-classical examples. In addition, the quiet but ubiquitous presence of symbolic manipulation systems provides a number of illustrations of the power of these systems while making it possible to test and concretely experiment with a great many combinatorial models. Symbolic systems allow for instance for fast random generation, close examination of non-asymptotic regimes, efficient experimentation with analytic expansions and singularities, and so on.

Our initial motivation when starting this project was to build a coherent set of methods useful in the analysis of algorithms, a domain of computer science now well-developed and presented in books by Knuth, Hofri, Mahmoud, and Szpankowski, in the survey by Vitter–Flajolet, as well as in our earlier *Introduction to the Analysis of Algorithms* published in 1996. This book, *Analytic Combinatorics*, can then be used as a systematic presentation of methods that have proved immensely useful in this area; see in particular the *Art of Computer Programming* by Knuth for background. Studies in statistical physics (van Rensburg, and others), statistics (e.g., David and Barton) and probability theory (e.g., Billingsley, Feller), mathematical logic (Burris' book), analytic number theory (e.g., Tenenbaum), computational biology (Waterman's textbook), as well as information theory (e.g., the books by Cover–Thomas, MacKay, and Szpankowski) point to many startling connections with yet other areas of science. The book may thus be useful as a supplementary reference on methods and applications in courses on statistics, probability theory, statistical physics, finite model theory, analytic number theory, information theory, computer algebra, complex analysis, or analysis of algorithms.

Acknowledgements. This book would be substantially different and much less informative without Neil Sloane's *Encyclopedia of Integer Sequences*, Steve Finch's *Mathematical Constants*, Eric Weisstein's *MathWorld*, and the *MacTutor History of Mathematics* site hosted at St Andrews. We have also greatly benefited of the existence of open on-line archives such as *Numdam*, *Gallica*, *GDZ* (digitalized mathematical documents), *ArXiv*, as well as the *Euler Archive*. All the corresponding sites are (or at least have been at some stage) freely available on the Internet. Bruno Salvy and Paul Zimmermann have developed algorithms and libraries for combinatorial structures and generating functions that are based on the MAPLE system for symbolic computations and that have proven to be extremely useful. We are deeply grateful to the authors of the free software Unix, Linux, Emacs, X11, TeX and LaTeX as well as to the designers of the symbolic manipulation system MAPLE for creating an environment that has proved invaluable to us. We also thank students in courses at Barcelona, Berkeley (MSRI), Bordeaux, Caen, Graz, Paris (École Polytechnique, École Normale Supérieure, University), Princeton, Santiago de Chile, Udine, and Vienna whose reactions have greatly helped us prepare a better book. Thanks finally to numerous colleagues for their contributions to this book project. In particular, we wish to acknowledge the support, help, and interaction provided at a high level by members of the *Analysis of Algorithms (AofA)* community, with a special mention for Nicolas Broutin, Michael Drmota, Éric Fusy, Hsien-Kuei Hwang, Svante Janson, Don Knuth, Guy Louchard, Andrew Odlyzko, Daniel Panario, Carine Pivoteau, Helmut Prodinger, Bruno Salvy, Michèle Soria, Wojtek Szpankowski, Brigitte Vallée, Mark Daniel Ward, and Mark Wilson. In addition, Ed Bender, Stan Burris, Philippe Dumas, Svante Janson, Philippe Robert, Loïc Turban, and Brigitte Vallée have provided insightful suggestions and generous feedback that have led us to revise the presentation of several sections of this book and correct many errors. We were also extremely lucky to work with David Tranah, the mathematics editor of Cambridge University Press, who has been an exceptionally supportive (and patient) companion of this book project, throughout all these years. Finally, support of our home institutions (INRIA and Princeton University) as well as various grants (French government, European Union, and NSF) have contributed to making our collaboration possible.

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An Invitation to Analytic Combinatorics

διὸ δὴ συμμειγνύμενα αὐτά τε πρὸς αὐτὰ καὶ πρὸς ἄλληλα τὴν
ποικιλίαν ἐστὶν ἄπειρα· ἧς δὴ δεῖ θεωροὺς γίγνεσθαι τοὺς
μέλλοντας περὶ φύσεως εἰκότι λόγῳ

— PLATO, The Timaeus[1]

ANALYTIC COMBINATORICS is primarily a book about *combinatorics*, that is, the study of finite structures built according to a finite set of rules. *Analytic* in the title means that we concern ourselves with methods from mathematical analysis, in particular complex and asymptotic analysis. The two fields, combinatorial enumeration and complex analysis, are organized into a coherent set of methods for the first time in this book. Our broad objective is to discover how the continuous may help us to understand the discrete and to *quantify* its properties.

COMBINATORICS is, as told by its name, the science of combinations. Given basic rules for assembling simple components, what are the properties of the resulting objects? Here, our goal is to develop methods dedicated to *quantitative* properties of combinatorial structures. In other words, we want to measure things. Say that we have n different items like cards or balls of different colours. In how many ways can we lay them on a table, all in one row? You certainly recognize this counting problem—finding the number of *permutations* of n elements. The answer is of course the factorial number

$$n\,! = 1 \cdot 2 \cdot \ldots \cdot n.$$

This is a good start, and, equipped with patience or a calculator, we soon determine that if $n = 31$, say, then the number of permutations is the rather large quantity

$$31\,! = 8222838654177922817725562880000000,.$$

an integer with 34 decimal digits. The factorials solve an enumeration problem, one that took mankind some time to sort out, because the sense of the "$\cdots$" in the formula for $n!$ is not that easily grasped. In his book *The Art of Computer Programming*

[1] *"So their combinations with themselves and with each other give rise to endless complexities, which anyone who is to give a likely account of reality must survey."* Plato speaks of Platonic solids viewed as idealized primary constituents of the physical universe.

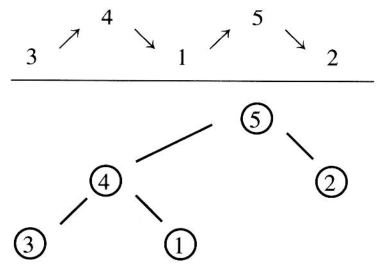

Figure 0.1. An example of the correspondence between an alternating permutation (top) and a decreasing binary tree (bottom): each binary node has two descendants, which bear smaller labels. Such *constructions*, which give access to *generating functions* and eventually provide solutions to counting problems, are the main subject of Part A.

(vol III, p. 23), Donald Knuth traces the discovery to the Hebrew *Book of Creation* (c. AD 400) and the Indian classic *Anuyogadvāra-sutra* (c. AD 500).

Here is another more subtle problem. Assume that you are interested in permutations such that the first element is smaller than the second, the second is larger than the third, itself smaller than the fourth, and so on. The permutations go up and down and they are diversely known as up-and-down or zigzag permutations, the more dignified name being *alternating* permutations. Say that $n = 2m + 1$ is odd. An example is for $n = 9$:

$$4 \nearrow 8 \searrow 6 \nearrow 7 \searrow 5 \nearrow 9 \searrow 1 \nearrow 3 \searrow 2$$

The number of alternating permutations for $n = 1, 3, 5, \ldots, 15$ turns out to be

$$1, 2, 16, 272, 7936, 353792, 22368256, 1903757312.$$

What are these numbers and how do they relate to the total number of permutations of corresponding size? A glance at the corresponding figures, that is, $1!, 3!, 5!, \ldots, 15!$, or

$$1, 6, 120, 5040, 362880, 39916800, 6227020800, 1307674368000,$$

suggests that the factorials grow somewhat faster—just compare the lengths of the last two displayed lines. But how and by how much? This is the prototypical question we are addressing in this book.

Let us now examine the counting of alternating permutations. In 1881, the French mathematician Désiré André made a startling discovery. Look at the first terms of the Taylor expansion of the trigonometric function $\tan z$:

$$\tan z = 1\frac{z}{1!} + 2\frac{z^3}{3!} + 16\frac{z^5}{5!} + 272\frac{z^7}{7!} + 7936\frac{z^9}{9!} + 353792\frac{z^{11}}{11!} + \cdots .$$

The counting sequence for alternating permutations, $1, 2, 16, \ldots$, curiously surfaces. We say that the function on the left is a *generating function* for the numerical sequence (precisely, a generating function of the *exponential* type, due to the presence of factorials in the denominators).

André's derivation may nowadays be viewed very simply as reflecting the construction of permutations by means of certain labelled binary trees (Figure 0.1 and p. 143): given a permutation σ a tree can be obtained once σ has been decomposed as a triple $\langle \sigma_L, \max, \sigma_R \rangle$, by taking the maximum element as the root, and appending, as left and right subtrees, the trees recursively constructed from σ_L and σ_R. Part A of this book develops at length *symbolic methods* by which the construction of the class $\mathcal{T}$ of all such trees,

$$\mathcal{T} \quad = \quad ① \quad \cup \quad (\mathcal{T}, \max, \mathcal{T}),$$

translates into an equation relating generating functions,

$$T(z) \quad = \quad z \quad + \quad \int_0^z T(w)^2\, dw.$$

In this equation, $T(z) := \sum_n T_n z^n/n!$ is the exponential generating function of the sequence (T_n), where T_n is the number of alternating permutations of (odd) length n. There is a compelling formal analogy between the combinatorial *specification* and its generating function: Unions ($\cup$) give rise to sums ($+$), max-placement gives an integral ($\int$), forming a pair of trees corresponds to taking a square ($[\cdot]^2$).

At this stage, we know that $T(z)$ must solve the differential equation

$$\frac{d}{dz}T(z) = 1 + T(z)^2, \qquad T(0) = 0,$$

which, by classical manipulations[2], yields the explicit form

$$T(z) = \tan z.$$

The generating function then provides a simple *algorithm* to compute the coefficients recurrently. Indeed, the formula,

$$\tan z = \frac{\sin z}{\cos z} = \frac{z - \frac{z^3}{3!} + \frac{z^5}{5!} - \cdots}{1 - \frac{z^2}{2!} + \frac{z^4}{4!} - \cdots},$$

implies, for n odd, the relation (extract the coefficient of z^n in $T(z)\cos z = \sin z$)

$$T_n - \binom{n}{2}T_{n-2} + \binom{n}{4}T_{n-4} - \cdots = (-1)^{(n-1)/2}, \quad \text{where} \quad \binom{a}{b} = \frac{a!}{b!(a-b)!}$$

is the conventional notation for binomial coefficients. Now, the exact enumeration problem may be regarded as solved since a very simple algorithm is available for determining the counting sequence, while the generating function admits an explicit expression in terms of well-known mathematical objects.

ANALYSIS, by which we mean mathematical analysis, is often described as the art and science of *approximation*. How fast do the factorial and the tangent number sequences grow? What about *comparing* their growths? These are typical problems of analysis.

[2]We have $T'/(1+T^2) = 1$, hence $\arctan(T) = z$ and $T = \tan z$.

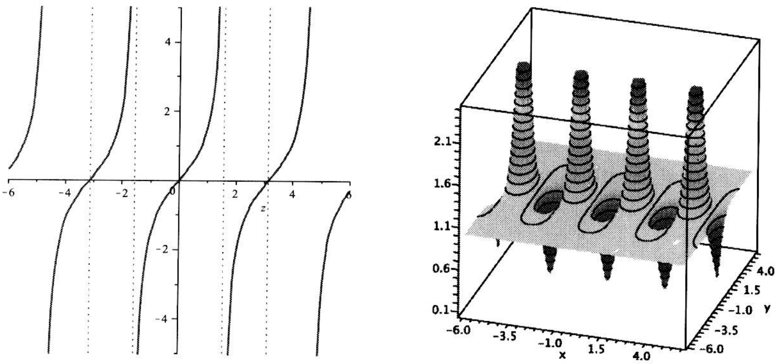

Figure 0.2. Two views of the function $z \mapsto \tan z$. Left: a plot for real values of $z \in [-6, 6]$. Right: the modulus $|\tan z|$ when $z = x + iy$ (with $i = \sqrt{-1}$) is assigned complex values in the square $\pm 6 \pm 6i$. As developed at length in Part B, it is the nature of *singularities* in the *complex domain* that matters.

First, consider the number of permutations, $n!$. Quantifying its growth, as n gets large, takes us to the realm of *asymptotic analysis*. The way to express factorial numbers in terms of elementary functions is known as Stirling's formula[3]

$$n! \sim n^n e^{-n} \sqrt{2\pi n},$$

where the $\sim$ sign means "approximately equal" (in the precise sense that the ratio of both terms tends to 1 as n gets large). This beautiful formula, associated with the name of the Scottish mathematician James Stirling (1692–1770), curiously involves both the basis e of natural logarithms and the perimeter 2π of the circle. Certainly, you cannot get such a thing without analysis. As a first step, there is an estimate

$$\log n! = \sum_{j=1}^{n} \log j \sim \int_1^n \log x \, dx \sim n \log\left(\frac{n}{e}\right),$$

explaining at least the $n^n e^{-n}$ term, but already requiring a certain amount of elementary calculus. (Stirling's formula precisely came a few decades after the fundamental bases of calculus had been laid by Newton and Leibniz.) Note the utility of Stirling's formula: it tells us almost instantly that 100! has 158 digits, while 1000! borders the astronomical 10^{2568}.

We are now left with estimating the growth of the sequence of tangent numbers, T_n. The analysis leading to the derivation of the generating function $\tan(z)$ has been so far essentially algebraic or "formal". Well, we can plot the graph of the tangent function, for real values of its argument and see that the function becomes infinite at the points $\pm\frac{\pi}{2}$, $\pm 3\frac{\pi}{2}$, and so on (Figure 0.2). Such points where a function ceases to be

[3] In this book, we shall encounter five different proofs of Stirling's formula, each of interest for its own sake: (*i*) by singularity analysis of the Cayley tree function (p. 407); (*ii*) by singularity analysis of polylogarithms (p. 410); (*iii*) by the saddle-point method (p. 555); (*iv*) by Laplace's method (p. 760); (*v*) by the Mellin transform method applied to the logarithm of the Gamma function (p. 766).