This book is the first complete presentation in English of the combinatorial theory of species, introduced by A. Joyal in 1980. It gives a unified understanding of the use of generating functions for both labeled and unlabeled structures as and also provides a tool for the specification and analysis of these structures. Of particular importance is the capacity of combinatorial species to transform recursive definitions of tree-like structures into functional or differential equations, and conversely.

Some of the features of this book are:

- A detailed analysis of classes of combinatorial structures such as permutations, total orders, graphs, trees, rooted trees, data structures, etc., including the basic constructions and operations that can be performed on them and on their various generating series.
- A thorough study of data structures defined by functional equations: binary trees, (2,3)-, (a,b)- and B-trees, AVL trees, PQ-trees, leftist trees, ordered rooted trees and many other classes of enriched rooted trees.
- Extensive discussions of various links between combinatorics and other parts of mathematics: orthogonal polynomials, Lagrange inversion formula, implicit function theorem, Newton–Raphson iteration, differential equations, symmetric functions, and asymptotic analysis.
- An extension of Pólya theory to classes of structures defined by combinatorial operations or by functional equations and to asymmetric structures.

This book will be a valuable reference to graduate students and researchers in combinatorics, analysis, probability theory, and theoretical computer science.

ENCYCLOPEDIA OF MATHEMATICS AND ITS APPLICATIONS

EDITED BY G.-C. ROTA

Volume 67

Combinatorial Species and Tree-like Structures

ENCYCLOPEDIA OF MATHEMATICS AND ITS APPLICATIONS

6 H. Minc *Permanents*
18 H. O. Fattorini *The Cauchy Problem*
19 G. G. Lorentz, K. Jetter, and S. D. Riemenschneider *Birkhoff Interpolation*
22 J. R. Bastida *Field Extensions and Galois Theory*
23 J. R. Cannon *The One-Dimensional Heat Equation*
24 S. Wagon *The Banach-Tarski Paradox*
25 A. Salomaa *Computation and Automata*
26 N. White (ed.) *Theory of Matroids*
27 N. H. Bingham, C. M. Goldie, and J. L. Teugels *Regular Variation*
28 P. P. Petrushev and V. P. Popov *Rational Approximation of Real Functions*
29 N. White (ed.) *Combinatorial Geometries*
30 M. Pohst and H. Zassenhaus *Algorithmic Algebraic Number Theory*
31 J. Aczel and J. Dhombres *Functional Equations in Several Variables*
32 M. Kuczma, B. Choczewski, and R. Ger *Iterative Functional Equations*
33 R. V. Ambartzumian *Factorization Calculus and Geometric Probability*
34 G. Gripenberg, S.-O. Londen and O. Staffans *Volterra Integral and Functional Equations*
35 G. Gasper and M. Rahman *Basic Hypergeometric Series*
36 E. Torgersen *Comparison of Statistical Experiments*
37 A. Neumaier *Interval Methods for Systems of Equations*
38 N. Korneichuk *Exact Constants in Approximation Theory*
39 R. A. Brualdi and H. Ryser *Combinatorial Matrix Theory*
40 N. White (ed.) *Matroid Applications*
41 S. Sakai *Operator Algebras in Dynamical Systems*
42 W. Hodges *Basic Model Theory*
43 H. Stahl and V. Totik *General Orthogonal Polynomials*
45 G. Da Prato and J. Zabczyk *Stochastic Equations in Infinite Dimensions*
46 A. Björner et al. *Oriented Matroids*
47 G. Edgar and L. Sucheston *Stopping Times and Directed Processes*
48 C. Sims *Computation With Finitely Presented Groups*
49 T. Palmer *Banach Algebras and the General Theory of *-Algebras*
50 F. Borceux *Handbook of Categorical Algebra 1*
51 F. Borceux *Handbook of Categorical Algebra 2*
52 F. Borceux *Handbook of Categorical Algebra 3*
54 A. Katok and B. Hasselblatt *Introduction to the Modern Theory of Dynamical Systems*
55 V. N. Sachkov *Combinatorial Methods in Discrete Mathematics*
56 V. N. Sachkov *Probabilistic Methods in Discrete Mathematics*
57 P. M. Cohn *Skew Fields*
58 Richard Gardner *Geometric Tomography*
59 George A. Baker Jr. and Peter Graves-Morris *Pade Approximants*
60 Jan Krajicek *Bounded Arithmetic, Propositional Logic and Complexity Theory*
61 H. Groemer *Geometric Applications of Fourier Series and Spherical Harmonics*
62 H. O. Fattorini *Infinite Dimensional Optimization and Control Theory*
63 A. C. Thompson *Minkowski Geometry*

ENCYCLOPEDIA OF MATHEMATICS AND ITS APPLICATIONS

Combinatorial Species and Tree-like Structures

F. BERGERON
Université du Québec à Montréal

G. LABELLE
Université du Québec à Montréal

P. LEROUX
Université du Québec à Montréal

Translated from French by Margaret Readdy

CAMBRIDGE
UNIVERSITY PRESS

PUBLISHED BY THE PRESS SYNDICATE OF THE UNIVERSITY OF CAMBRIDGE
The Pitt Building, Trumpington Street, Cambridge CB2 1RP, United Kingdom

CAMBRIDGE UNIVERSITY PRESS
The Edinburgh Building, Cambridge CB2 2RU, United Kingdom
40 West 20th Street, New York, NY 10011-4211, USA
10 Stamford Road, Oakleigh, Melbourne 3166, Australia

French edition:
Théroie des espèces et combinatoire des structures arborescentes,
Publications du LACIM, vol. 19, 1994

First published in English in 1998

Typeset in Times

Library of Congress Cataloging-in-Publication Data

Bergeron, F.
[Théorie des espèces et combinatoire des structures arborescentes. English]
Combinatorial species and tree-like structures / F. Bergeron, G. Labelle, P. Leroux: translated from the French by Margaret Readdy.
p. cm. – (Encyclopedia of mathematics and its applications; v. 67)
Includes bibliographical references (p. –) and index.
ISBN 0-521-57323-8 (hardback)
1. Combinatorial enumeration problems. I. Labelle, Gilbert, 1944– . II. Leroux, P. (Pierre). 1942– . III. Title. IV. Series.
QA164.8.B4713 1997 96-46136
511′.5—dc20 CIP

A catalog record for this book is available from the British Library

ISBN 0 521 57323 8 hardback

Transferred to digital printing 2004

Foreword

by Gian-Carlo Rota

Advances in mathematics occur in one of two ways.

The first occurs by the solution of some outstanding problem, such as the Bieberbach conjecture or Fermat's conjecture. Such solutions are justly acclaimed by the mathematical community. The solution of every famous mathematical problem is the result of joint effort of a great many mathematicians. It always comes as an unexpected application of theories that were previously developed without a specific purpose, theories whose effectiveness was at first thought to be highly questionable.

Mathematicians realized long ago that it is hopeless to get the lay public to understand the miracle of unexpected effectiveness of theory. The public, misled by two hundred years of Romantic fantasies, clamors for some "genius" whose brain power cracks open the secrets of nature. It is therefore a common public relations gimmick to give the entire credit for the solution of famous problems to the one mathematician who is responsible for the last step.

It would probably be counterproductive to let it be known that behind every "genius" there lurks a beehive of research mathematicians who gradually built up to the "final" step in seemingly pointless research papers. And it would be fatal to let it be known that the showcase problems of mathematics are of little or no interest for the progress of mathematics. We all know that they are dead ends, curiosities, good only as confirmation of the effectiveness of theory. What mathematicians privately celebrate when one of their showcase problems is solved is Polya's adage: "no problem is ever solved directly."

There is a second way by which mathematics advances, one that mathematicians are also reluctant to publicize. It happens whenever some commonsense notion that had heretofore been taken for granted is discovered to be wanting, to need clarification or definition. Such foundational advances produce substantial dividends, but not right away. The usual accusation that is leveled against mathematicians who dare propose overhauls of the obvious is that of being "too abstract." As if one piece of mathematics could be "more abstract" than another, except in the eyes of the beholder (it is time to raise a cry of alarm against the misuse of the word "abstract," which has become as meaningless as the word "Platonism.")

An amusing case history of an advance of the second kind is uniform convergence, which first made headway in the latter quarter of the nineteenth century. The late Herbert Busemann told me that while he was a student, his analysis teachers admitted their inability to visualize uniform convergence, and viewed it as the outermost limit of abstraction. It took a few more generations to get uniform convergence taught in undergraduate classes.

The hostility against groups, when groups were first "abstracted" from the earlier "group of permutations" is another case in point. Hadamard admitted to being unable to visualize groups except as groups of permutations. In the thirties, when groups made their first inroad into physics via quantum mechanics, a staunch sect of reactionary physicists, repeatedly cried "Victory!" after convincing themselves of having finally rid physics of the "Gruppenpest." Later, they tried to have this episode erased from the history of physics.

In our time, we have witnessed at least two displays of hostility against new mathematical ideas. The first was directed against lattice theory, and its virulence all but succeeded in wiping lattice theory off the mathematical map. The second, still going on, is directed against the theory of categories. Grothendieck did much to show the simplifying power of categories in mathematics. Categories have broadened our view all the way to the solution of the Weil conjectures. Today, after the advent of braided categories and quantum groups, categories are beginning to look downright concrete, and the last remaining anticategorical reactionaries are beginning to look downright pathetic.

There is a common pattern to advances in mathematics of the second kind. They inevitably begin when someone points out that items that were formerly thought to be "the same" are not really "the same," while the opposition claims that "it does not matter," or "these are piddling distinctions." Take the notion of species that is the subject of this book. The distinction between "labeled graphs" and "unlabeled graphs" has long been familiar. Everyone agrees on the definition of an unlabeled graph, but until a while ago the notion of labeled graph was taken as obvious and not in need of clarification. If you objected that a graph whose vertices are labeled by cyclic permutations – nowadays called a "fat graph" – is not the same thing as a graph whose vertices are labeled by integers, you were given a strange look and you would not be invited to the next combinatorics meeting.

The correct definition of a labeled graph turned out to be more sophisticated than the definition of an unlabeled graph. A labeled graph – or any "labeled" combinatorial construct – is a functor from the groupoid of finite sets and bijections to itself. This definition of a labeled object is not "abstract": on the contrary, it expresses in precise terms the commonsense idea of "being able to label the vertices of a graph either by integers or by colors, it does not matter," and it is the only way of making this commonsense idea precise. The notion of groupoid, which is one of the key ideas of contemporary mathematics, makes it possible to withhold the assignement of a specific set of labels to the vertices of a graph without making the graph unlabeled.

Joyal's definition of "labeled object" as a species discloses a vast horizon of new combinatorial constructions, which cannot be seen if one holds on to the reactionary view that "labeled objects" need no definition. The simplest, and the most remarkable, application of the definition of species is the rigorous combinatorial rendering of functional composition, which was formerly dealt with by handwaving – always a bad sign. But it is just the beginning.

Species are related to generating functions in much the same way as random variables are related to probability distributions. Those probabilists of the thirties who held on to distributions, while rejecting random variables as "superfluous," were eventually wiped out, and their results are not even acknowledged today.

I dare make a prediction on the future acceptance of this book. At first, the old fogies will pretend the book does not exist. This pretense will last until sufficiently many younger combinatorialists publish papers in which interesting problems are solved using the theory of species. Eventually, a major problem will be solved in the language of species, and from that time on everyone will have to take notice. The rewriting, copying and imitating will start, and mathematicians who capitulate to the new theory will begin to tell us what species really are. Considering the speed at which mathematics progresses in our day, that time is more likely to come sooner than later.

The present book is the first thorough treatment in English of the theory of species. It is lucidly and clearly written, and it should go a long way to making this fundamental chapter of combinatorial mathematics available to the entire spectrum of mathematicians, computer scientists and cultivated scientists generally.

Cambridge, April 27, 1997

Table of Contents

Foreword *page* v
Preface xi

1 Introduction to Species of Structures 1
1.0 Introduction 1
1.1 Notion of Species of Structures 1
1.2 Associated Series 12
1.3 Addition and Multiplication 26
1.4 Substitution and Differentiation 40

2 Complements on Species of Structures 59
2.0 Introduction 59
2.1 Pointing and Cartesian Product 60
2.2 Functorial Composition 70
2.3 Weighted Species 79
2.4 Extension to the Multisort Context 100
2.5 Virtual Species 120
2.6 Molecular and Atomic Species 139

3 Combinatorial Functional Equations 162
3.0 Introduction 162
3.1 Lagrange Inversion 164
3.2 Implicit Species Theorem 191
3.3 Quadratic Iterative Methods 222
3.4 Elements of Asymptotic Analysis 247

4 Complements on Unlabeled Enumeration 277
4.0 Introduction 277
4.1 The Dissymmetry Theorem for Trees 278

4.2 Connected Graphs and Blocks 297
4.3 Proof of the Substitution Formulas 309
4.4 Asymmetric Structures 321

5 Species on Totally Ordered Sets 341
5.0 Introduction 341
5.1 $\mathbb{L}$-Species 342
5.2 Combinatorial Differential Equations 358

Appendix 1: Group Actions and Pólya Theory 393
Appendix 2: Miscellaneous Tables 408
Bibliography 434
Notation Indexx 447
Index 449

Preface

During the last decades considerable progress has been made in clarifying and strengthening the foundation of enumerative combinatorics. A number of useful theories, especially to explain algebraic techniques, have emerged. We mention, among others, *Möbius inversion* (Rota [284], Rota–Smith [289], Rota–Sagan [288]), *partitional composition* (Cartier–Foata [45], Foata [106, 112]), *prefabs* (Bender–Goldman [11]), *reduced incidence algebras* (Mullin–Rota [253], Doubilet, Rota, and Stanley [80], Dür [84]), *binomial posets* and *exponential structures* (Stanley [301, 300]), *Möbius categories* (Content–Lemay–Leroux [66], Leroux [212, 214]), *umbral calculus* and *Hopf algebras* (Rota [286], Joni–Rota [157]), *Pólya theory* (Pólya [263], Redfield [275], de Bruijn [68], Robinson [282]), and *species of structures* (Joyal [158]). Many authors have also underlined the importance of these methods to solve problems of enumeration, in particular, Bender–Williamson [12], Berge [13], Comtet [58], Flajolet [91], Goulden–Jackson [133], Graham–Knuth–Patashnik [136], Kerber [169], Harary–Palmer [144], Knuth [172], Liu [222], Riordan [281], Moon [251], Sagan [290], Stanley [304, 302], Stanton–White [306], van Lint–Wilson [316], Wehrhahn [324], and Wilf [326].

In addition, during this same period, the subject has been greatly enriched by its interaction with theoretical computer science as a source of application and motivation. The importance of combinatorics for the analysis of algorithms and the elaboration of efficient data structures is established in the fundamental book of Knuth [172]. A good knowledge of combinatorics is now essential to the computer scientist. Of particular importance are the following areas: formal languages, grammars, and automata theory (see for instance Berstel–Reutenauer [30], Eilenberg [88], Greene [137], Lothaire [227], Reutenauer [276, 277], and the work of Schützenberger, Cori, Viennot and the Bordeaux School); asymptotic analysis and average case complexity (see Bender [9], Bender–Canfield [10], Flajolet–Odlyzko [97], Flajolet–Salvy–Zimmermann [99], Knuth [172], and Sedgewick–Flajolet [295]); and combinatorics of data structures (see Aho–Hopcroft–Ullman

[1], Baeza-Yates–Gonnet [5], Brassard–Bratley [38], Mehlhorn [244], and Williamson[329]).

The combinatorial theory of species, introduced by Joyal in 1980, is set in this general framework. It provides a unified understanding of the use of generating series for both labeled and unlabeled structures, as well as a tool for the specification and analysis of these structures. Of particular importance is its capacity to transform recursive definitions of (tree-like) structures into functional or differential equations, and conversely. Encompassing the description of structures together with permutation group actions, the theory of species conciliates the calculus of generating series and functional equations with Pólya theory, following previous efforts to establish an algebra of cycle index series, particularly by de Bruijn [68] and Robinson [282]. This is achieved by extending the concept of group actions to that of functors defined on groupoids, in this case the category of finite sets and bijections. The functorial concept of species of structures goes back to Ehresmann [87]. The functorial property of combinatorial constructions on sets is also pointed out in a paper of Mullin and Rota [253] in the case of reluctant functions, a crucial concept for the combinatorial understanding of Lagrange inversion. There are also links between the algebra of operations on species and category theory. For example, the partitional composition of species can be described in the general settings of doctrines (see Kelly [166]), operads (see May [233] and Loday [224]), and analytic functors (see Joyal [163]).

Informally, a species of structures is a rule, F, associating with each finite set U, a finite set $F[U]$ which is "independent of the nature" of the elements of U. The members of the set $F[U]$, called *F-structures*, are interpreted as combinatorial structures on the set U given by the rule F. The fact that the rule is independent of the nature of the elements of U is expressed by an invariance under relabeling. More precisely, to any bijection $\sigma : U \longrightarrow V$, the rule F associates a bijection $F[\sigma] : F[U] \longrightarrow F[V]$ which transforms each F-structure on U into an (isomorphic) F-structure on V. It is also required that the association $\sigma \mapsto F[\sigma]$ be consistent with composition of bijections. In this way the concept of species of structures puts as much emphasis on isomorphisms as on the structures themselves. In categorical terms, a species of structures is simply a functor from the category $\mathbb{B}$ of finite sets and bijections to itself.

As an example, the class $\mathcal{G}$ of simple (finite) graphs and their isomorphisms, in the usual sense, give rise to the species of graphs, also denoted $\mathcal{G}$. For each set U, the elements of $\mathcal{G}[U]$ are just the simple graphs with vertex set U. For each $\sigma : U \longrightarrow V$, the bijection $\mathcal{G}[\sigma] : \mathcal{G}[U] \longrightarrow \mathcal{G}[V]$ transforms each simple graph on U into a graph on V by relabeling via σ. Similarly, any class of discrete structures closed under isomorphisms gives rise to a species.

Furthermore, species of structures can be combined to form new species by using set theoretical constructions. There results a variety of combinatorial operations on species, including addition, multiplication, substitution, derivation, etc., which extend the familiar calculus of formal power series. Indeed to each species of structures, we can associate various formal power series designed to treat enumeration problems of a specific kind (labeled, unlabeled, asymmetric, weighted, etc.). Of key importance is the fact that these associated series are "compatible" with operations on species. Hence each (algebraic, functional, or differential) identity between species implies identities between their associated series. This is in the spirit of Euler's method of generating series.

For example, let $\mathfrak{a}$ denote the species of *trees* (acyclic connected simple graphs) and $\mathcal{A}$, that of *rooted trees* (trees with a distinguished vertex). Then the functional equation

$$\mathcal{A} = XE(\mathcal{A}), \tag{1}$$

expresses the basic fact that any rooted tree on a finite set U can be naturally described as a root (a vertex $x \in U$) to which is attached a set of disjoint rooted trees (on $U \setminus \{x\}$); see Figure 1.4.4. Equation (1) yields immediately the following equalities between generating series

$$\mathcal{A}(x) = xe^{\mathcal{A}(x)}, \qquad T(x) = x \exp\left(\sum_{k\geq 0} \frac{T(x^k)}{k}\right). \tag{2}$$

These formulas go back to Cayley [46] and Pólya [263]. The first refers to the exponential generating series $\mathcal{A}(x) = \sum_{n\geq 0} a_n x^n/n!$, where a_n is the number of rooted trees on a set of n elements (labeled rooted trees), and yields Cayley's formula $a_n = n^{n-1}$ via the Lagrange inversion formula. The second refers to the ordinary generating series $T(x) = \sum_{n\geq 0} T_n x^n$, where T_n is the number of isomorphism types of rooted trees (unlabeled rooted trees) on n elements, and yields a recurrence formula for these numbers (see 4.1.44).

Analogously, the identity

$$2(n-1)n^{n-2} = \sum_{k=1}^{n-1} \binom{n}{k} k^{k-1}(n-k)^{n-k-1}, \tag{3}$$

and Otter's formula [259]

$$t(x) = T(x) + \frac{1}{2}(T(x^2) - T^2(x)), \tag{4}$$

where $t(x) = \sum_{n\geq 1} t_n x^n$ is the ordinary generating series of the number t_n of unlabeled trees on n elements, both follow from the species isomorphism

$$\mathcal{A} + E_2(\mathcal{A}) = \mathfrak{a} + \mathcal{A}^2, \tag{5}$$

allowing us to express the species $\mathfrak{a}$ of trees as a function of the species of rooted trees. We call this identity the *dissymetry* theorem for trees (see Leroux [213], Leroux and Miloudi [215]). It is inspired from the dissimilarity formula of Otter

[259] and the work of Norman [257] and Robinson [282] on the decomposition of graphs into 2-connected components.

Since its introduction, the theory of species of structures has been the focus of considerable research by the Montréal school of combinatorics as well as numerous other researchers. The goal of this book is to present the basic elements of the theory and to give a unified account of some of it's developments and applications.

Chapter 1 contains the first key ideas of the theory. A general discussion on the notion of discrete structures leads naturally to the formal definition of species of structures. Some of the basic formal power series associated to a species F are introduced: the (exponential) generating series $F(x)$ for labeled enumeration, the type generating series $\widetilde{F}(x)$ for unlabeled enumeration, and the cycle index series $Z_F(x_1, x_2, x_3, \ldots)$ as a general enumeration tool. Finally, we introduce the combinatorial operations of addition, multiplication, substitution (partitional composition), and derivation of species of structures. These operations extend and interpret in the combinatorial context of species the corresponding operations on formal power series.

The second chapter begins with an introduction to three other operations: pointing, Cartesian product and functorial composition. Pointing is a combinatorial analogue of the operator $x(d/dx)$ on series. The Cartesian product, consisting of superposition of structures, corresponds to the *Hadamard product* of series (coefficientwise multiplication). Functorial composition, not to be confused with substitution, is the natural composition of species considered as functors (see Décoste–Labelle–Leroux [74]). Many species of graphs and multigraphs can be expressed easily by this operation.

The theory is then extended to weighted species where structures are counted according to certain parameters, and to multisort species in analogy with functions of several variables. These generalizations broaden the range of applications to more refined enumeration problems.

For example, the generating series for Laguerre polynomials,

$$\sum_{n\geq 0} \mathcal{L}_n^{(\alpha)}(t)\frac{x^n}{n!} = \left(\frac{1}{1-x}\right)^{\alpha+1} \exp\left(\frac{-tx}{1-x}\right), \tag{6}$$

suggests a combinatorial "model" for these polynomials, consisting of permutations (with cycle counter $\alpha + 1$) and oriented chains (each with weight $-t$). This model gives rise to a combinatorial theory of Laguerre polynomials, where identities appear as consequences of elementary constructions on discrete structures. The same approach can be applied to many other families of polynomials. See, for example, Bergeron [20], Dumont [83], Foata [107, 109], Foata–Labelle [110], Foata–Leroux [111], Foata–Schützenberger [112], Foata–Strehl [113, 114], Foata–Zeilberger [115], Labelle–Yeh [202, 204, 208], Leroux–Strehl [216], Strehl [308, 309, 310], Viennot [319], and Zeng [340]. Following those lines, the book contains a combinatorial treatment of Eulerian, Hermite, Laguerre, and Jacobi polynomials.

Finally Chapter 2 introduces *virtual* species due to Joyal [162, 161] and Yeh [333, 334], making possible the subtraction of species, and develops an analysis of *molecular* (indecomposable with respect to addition) and *atomic* (indecomposable with respect to both addition and multiplication) species. These tools allow the construction of a multiplicative inverse $1/F$, for species F such that $F(0) = 1$, as well as the construction of an inverse for substitution $G^{\langle -1\rangle}$, for species G such that $G(0) = 0$ and $G'(0) = 1$.

Chapter 3 is concerned with a deeper study of the combinatorial functional equation

$$Y = XR(Y), \tag{7}$$

related to Lagrange inversion, as well as of more general equations of the form

$$Y = H(X, Y), \tag{8}$$

or even $Y = H(X, Y \circ G)$, where R, H, and G are given species, and Y is the unknown. The combinatorial resolution of these equations gives rise to tree-like structures that can be described recursively. In particular, the solution of the functional equation $Y = XR(Y)$ is a species of structures consisting of rooted trees whose fibers are "enriched" (or "structured") by the species R. The enumeration of these structures by combinatorial means leads to a combinatorial proof of the classical Lagrange inversion formulas (see Labelle [178] and Joyal [158]). Another proof of Lagrange inversion, also based on enriched rooted trees, is given by Chen [48, 51]. The enumeration of enriched rooted trees also leads to binomial type sequences naturally associated with the series $R(x)$ (see Rota [286]).

The more general equation $Y = H(X, Y)$, $Y(0) = 0$, is then considered. We give sufficient conditions for the existence and "uniqueness" of combinatorial solutions of systems of equations of this type. In particular, a multidimensional Lagrange inversion formula is established, following the approach of Gessel [127], which is then applied to the calculation of the index series of R-enriched rooted trees (see Décoste–Labelle–Leroux [73] and Labelle [181]).

The iterative method of Newton–Raphson for the solution of functional equations has a natural analogue in the context of species of structures (see Décoste–Labelle–Leroux [73] and Labelle [181]). It yields an iterative process with "quadratic convergence" for calculating species of structures defined by equations of the form $Y = XR(Y)$ or of the form

$$Y = X + G(Y), \tag{9}$$

where G is a given species, or more generally of the form $Y = H(X, Y)$. Functional equations of type

$$Y = H(X, Y \circ G), \tag{10}$$

which we call *Read–Bajraktarević* equations, lend themselves to an iterative approach and are also treated here (see Bergeron–Labelle–Leroux [23]). This work is motivated, from the point of view of computer science, by the complexity analysis of update algorithms for various kind of "balanced trees" for which equation (10) arises naturally.

This chapter concludes with an overview of various techniques of asymptotic analysis applied to the enumeration of F-structures on $\{1, 2, \ldots, n\}$ as $n \to \infty$. We give particular attention to the case of tree-like structures. The main methods considered are the analysis of dominant singularities, the method of Hayman (singularity at infinity), a theorem of Meir and Moon [234, 241] on the equation $y = xR(y)$, and one of Bender [9] on the equation $y = H(x, y)$.

Chapter 4 is devoted to a more thorough analysis of unlabeled enumeration. For species of structures, this often involves calculation of their cycle index series and the establishment of functional equations between them. The case of (enriched) trees and rooted trees is treated in detail, including the dissymetry theorem for trees and its corollary, Otter's formula. We also study classes of simple graphs, for example, those whose *blocks* (2-connected components) belong to a given family (see Hanlon–Robinson [141]).

An objective of Chapter 4 is the detailed proof of the substitution formulas for weighted species, which are essential tools for unlabeled enumeration:

$$\widetilde{F_v \circ G_w}(x) = Z_{F_v}(\widetilde{G_w}(x), \widetilde{G_{w^2}}(x^2), \ldots), \tag{11}$$

$$Z_{F_v \circ G_w} = Z_{F_v}(Z_{G_w}(x_1, x_2, x_3, \ldots), Z_{G_{w^2}}(x_2, x_4, x_6, \ldots), \ldots). \tag{12}$$

This last formula generalizes both the theorem of Pólya for the wreath product of group actions (see Pólya [263], Section 27) and the composition theorem of Robinson for graphs (see Harary–Palmer [144], Chapter 8). The proofs given here of these formulas are based on the notion of wreaths of G-structures (see Joyal [158]) and on the algebraic independence of *power sum* symmetric functions

$$p_n = t_1^n + t_2^n + t_3^n + \cdots, \tag{13}$$

following the approach of Pólya. Substitution formula (12) describes the relation between "partitional composition" of species and plethysm of symmetric functions. Indeed, to any species of structures F corresponds a family of set-theoretical (linear) representations of the symmetric groups $\mathcal{S}_n$, $n \geq 0$. The symmetric function $Z_F(p_1, p_2, p_3, \ldots)$ is then the Frobenius characteristic of these representations and formula (12) reflects the fact that the characteristic of the composite of two representations is the plethysm of their characteristics (see Macdonald [228], Appendix A).

The last section of Chapter 4 is devoted to the study of *asymmetric* structures, that is, structures whose stabilizer reduces to the identity permutation. This problem has been solved, in the context of group actions, by Rota (in 1968) who introduced an acyclic indicator polynomial using Möbius inversion in the lattice of periods of the group action (see [285, 288, 289]). Asymmetric structures can also be studied in the general context of enumeration according to stabilizers, using Möbius inversion in the lattice of subgroups of a permutation group (see Stockmeyer [307], White [325], Kerber–Thürlings [171]). Following Pólya [263, Section 23], Harary–Prins [146], and Rota, our main tool for the enumeration of asymmetric structures is the *asymmetry index series* $\Gamma_F(x_1, x_2, x_3, \ldots)$ of a species F, which plays an analoguous role for this problem as the cycle index series Z_F for the enumeration of isomorphism types. In particular, as shown by G. Labelle [186], the assignment $F \mapsto \Gamma_F$ transforms combinatorial identities on species into corresponding functional and differential equations on asymmetry index series. For a unified presentation in the context of *Möbius species*, see Yang [331]. The series Z_F and Γ_F also give rise to canonical q-series induced by principal specialization (see Décoste [70, 71], Décoste–Labelle [72]).

In enumerative and algebraic combinatorics, structures often involve a given total (linear) order on the underlying set. Good examples are provided by alternating permutations or Young standard tableaux. Similarly, in computer science, data structures often make use of some explicit order on the set of data, as in the case of searching or sorting algorithms. To better deal with such constructions, we develop in Chapter 5 a variant of the theory of species of structures, the $\mathbb{L}$-*species*, where structures are supported by sets with a given total order. In this context, the differential equation

$$Y' = R(Y), \qquad Y(0) = 0, \tag{14}$$

admits a natural combinatorial solution which can be expresssed in terms of *increasing* enriched rooted trees.

We develop, in the context of $\mathbb{L}$-species, a combinatorial theory of autonomous and nonautonomous differential equations. See Leroux and Viennot [217, 218, 219, 220], and also Bergeron–Flajolet–Salvy [22], Bergeron–Reutenauer [26, 27], Rawlings [270], and Unger [315]. In particular, classical results (Lie–Gröbner–Taylor expansions, linear differential equations, the method of separation of variables) are analyzed from a combinatorial viewpoint. An application is given in the exercises to the generic solution (with computer algebra techniques) of differential equations occurring in control theory, for example, Duffing equation.

This book has two intended audiences: graduate students and researchers in pure and applied mathematics and computer science. It can be used as a graduate text in enumerative and algebraic combinatorics. The only prerequisites are a good knowledge of basic algebra and analysis and some familiarity with discrete mathematics. It offers a modern introduction to the use of various generating functions in labeled and unlabeled enumeration. The professional researcher in the areas of combinatorics, algebra, analysis, computer science, and probability theory will find combinatorial tools to solve problems occurring in their field.

This book has the following special features:

- A comprehensive presentation of the combinatorial theory of species of structures.
- A clear explanation of when to use the different types of generating series (ordinary, exponential, multivariate, cycle index, asymmetry index, molecular, etc.).
- An extensive study of combinatorial functional and differential equations and their relations with tree-like structures.
- Efficient tools for construction, analysis, classification, and enumeration of various species of discrete structures.
- A review of the connections between the theory of species and algebra via Möbius inversion; symmetric functions; finite group actions; molecular, atomic, and virtual species; and Pólya theory.
- Detailed discussion of various links between combinatorics and classical analysis: families of (orthogonal) polynomials, q-series, Lagrange inversion, implicit function theorem, Newton–Raphson iteration, functional and differential equations, asymptotic analysis, etc.
- Extended reference tools: numerous tables (see Appendix 2), a notation index, a general index, and a bibliography.

Finally, the book contains more than 350 exercises ranging from very easy (e.g., routine computations based on definitions, direct applications of theorems, ...) to very elaborate or difficult (e.g., step by step development of a topic not covered in the text, delicate analysis of hidden properties of complex species of stuctures, ...). They are found at the end of each section and serve as a complement to the theory as well as a "hands on" practice. Accordingly, the statements in most exercises are intentionally very explicit and can often be thought of as "theorems" to be proved. For instance, instead of asking to find a formula in a given context, an exercise may ask to prove (or verify) that an "explicitly stated" formula is true. The most difficult exercises are not really meant to be solved but should be read in order to have a more complete view of the theory and its applications.

Due to space and time limitations, some of the recent and interesting work related to species theory has not been covered in this book. The most notable omissions concern

- Connections with symmetric functions, λ-rings, and binomial rings. See, for instance, Bergeron [17, 18], Bonetti–Rota–Senato–Venezia [32, 33], Flores de Chela–Méndez [105], Joyal [159, 160], Kerber [170], Méndez [246], Nava [255], Senato–Venezia [296], and Yeh [333, 334].
- Extensions to tensorial species and analytic functors, and connections with group representations. See Bergeron–Yeh [29], Joyal [163], Joyal–Street [164], Macdonald [228], and Méndez [245].
- Colored and Möbius species. See Ehrenborg–Méndez [86], Méndez–Nava [247], Méndez–Yang [248], and Yang [331, 332].

- Connections with category theory, Hopf algebras, and umbral calculus. See Chen [49, 50, 51], Dür [84], Loeb [225], Nava–Rota [256], Rajan [267, 268], Ray [272], and Schmitt [292].
- Further developments and applications of species theory. See, for example, Bergeron [14, 19], Bergeron–Sattler [28], Chen [48, 51], Chiricota [53], Chiricota–Labelle [55], Constantineau [59, 61], Constantineau–Labelle [65], Gessel [128], Gessel–Labelle [129], Labelle [182, 184, 185], Labelle–Labelle–Pineau [190], Labelle–Laforest [192], Labelle–Yeh [203, 206], Longtin [226], Pineau [262], Strehl [311, 312], Unger [315], and Yeh [335].

Acknowledgments

We wish to warmly thank all the people who helped us during the preparation of this work and in particular, at the risk of forgetting someone, the following people:

- André Joyal, for having founded the combinatorial theory of species of structures and shown its importance in enumerative and algebraic combinatorics.
- Jean Berstel, for having realized the interest of species of structures in computer science and encouraged the creation of this book.
- Gian-Carlo Rota, for his constant interest in the theory of species and for inviting us to publish the English version of the book in this collection.
- The researchers and collaborators who have been interested in the theory of species of structures and who have participated in its development, including P. Bouchard, Ph. Flajolet, I. Gessel, A. Kerber, J. Labelle, L. Laforest, A. Longtin, D. Rawlings, C. Reutenauer, R.W. Robinson, G.-C. Rota, B. Salvy, S. Schanuel, R.P. Stanley, V. Strehl, G.X. Viennot, T. Walsh, K.H. Wehrhahn, Y.N. Yeh, and D. Zeilberger; as well as D. Foata, A. Garsia, J. Françon, G. Nicoletti, R.C. Read, B. Sagan, D. Stanton, D. White, H.S. Wilf, and A. Zvonkin.
- Young researchers whose dissertations dealt with species of structures, including W.C. Chen, Y. Chiricota, I. Constantineau, H. Décoste, R. Ehrenborg, M. Mendez, O. Nava, K. Pineau, B. Unger, and J. Yang.
- All the students and other colleagues who have read various versions of this book and have made comments and suggestions, including P. Auger, N. Bergeron, M. Bousquet, A. de Medicis, P. Dumais, L. Favreau, J.F. Gagné, A. Goupil, J. Labelle, J.B. Lévesque, G. Melançon, B. Miloudi, A. Nickel, S. Poirier, M. Poulin, E. Roblet, J. Roger, L. Shapiro, and J. Turgeon.
- Margaret Readdy for translating the book from French to English.
- For their more specific aid for
  typing and linguistic corrections: G. Hetyei, L. Remon, and A. Robitaille
  preparation of tables: Y. Chiricota, H. Décoste, M. Ikollo, J. Labelle, and K. Pineau
  preparation of index: A. Robitaille and F. Strasbourg
  preparation of figures: B. Girard and S. Plouffe.

- For their financial support, the Université du Québec à Montréal and the funding councils Fonds pour la formation de chercheurs et l'aide à la recherche (FCAR), Québec, and National Science and Engineering Research Council (NSERC), Canada.
- And above all, for their patience, understanding, and constant encouragement, our life companions Rosamaria, Hélène, and Madeleine.