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Introduction to

EXPERIMENTAL MATHEMATICS

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Introduction to Experimental Mathematics

Mathematics is not, and never will be, an empirical science, but mathematicians are finding that the use of computers and specialized software allows the generation of mathematical insight in the form of conjectures and examples, which pave the way for theorems and their proofs. In this way, the experimental approach to pure mathematics is revolutionizing the way research mathematicians work.

As the first of its kind, this book provides material for a one-semester course in experimental mathematics that will give students the tools and training needed to systematically investigate and develop mathematical theory using computer programs written in Maple. Accessible to readers without prior programming experience, and using examples of concrete mathematical problems to illustrate a wide range of techniques, the book gives a thorough introduction to the field of experimental mathematics, which will prepare students for the challenge posed by open mathematical problems.

Søren Eilers is a professor of mathematics at the University of Copenhagen, who heads the VILLUM Foundation Network for Experimental Mathematics in Number Theory, Operator Algebras, and Topology. He has received numerous teaching prizes as well as an outreach prize for developing the mathematics of LEGO, and is an expert of the classification of C*-algebras.

Rune Johansen was the first postdoc in experimental mathematics in Denmark, specializing in symbolic dynamics.

Preface

Mathematics is not, and never will be, an empirical science, but mathematicians are finding that the use of computers and specialized software allows the generation of mathematical insight in the form of conjectures and examples that pave the way for theorems and their proofs. In this way, the experimental approach to pure mathematics is revolutionizing the way research mathematicians work.

However, research mathematicians who take to experimentation are largely self-taught, both in the use of various software packages and when it comes to designing useful experiments, and the rapid growth of the use of experimentation in the formulation and development of mathematical theory has not been accompanied by a corresponding development of courses and textbooks. It is our immodest ambition to change that situation with this textbook.

About This Book

Being largely self-taught experimental mathematicians ourselves, we originally adopted an experimental approach to the teaching of experimental mathematics, and the book has evolved by trial and error for more than a decade in the form of lecture notes for various courses taught at the University of Copenhagen.

Like our courses, the book is aimed at beginning graduate students and advanced undergraduate students in mathematics. We assume that the reader has a corresponding general level of mathematical maturity, including knowledge of calculus, analysis, and linear algebra corresponding to the curriculum covered by standard introductory courses. A few isolated examples and exercises in the book require command of more advanced mathematical topics, but these instances are clearly marked and can be skipped with no hidden consequences.

Whereas we know of no textbook with similar ambitions to this one, there is a rich and beautiful literature aimed at the more accomplished mathematician, discussing the philosophy of experimentation in mathematics and establishing by generous collections of examples how and why experimental mathematics should be done. Standing very much on the shoulders of the giants who pioneered the field of experimental mathematics, we have incorporated the work of many of these in the book as worked examples or exercises. As will be obvious from the remarks closing each chapter, we are particularly indebted to the works of David Bailey, Jonathan Borwein, Peter Borwein, and Doron Zeilberger.

For the Student

Experimental mathematics is not a spectator sport, even less so than traditional pure mathematics. As a consequence, this book contains fewer theorems and more examples than a traditional mathematics textbook. It is of paramount importance that you immerse yourself in these and try your hand at conducting small- to medium-scale experiments as you read through the book, especially if you are using this book for self-study. In a traditional mathematical textbook, examples and exercises are crucial for grasping difficult theoretical content, but to some extent, they can be seen as the means to an end: the goal is to understand the theory. In this book, on the other hand, examples and exercises constitute the backbone of the learning process, whereas the general explanations and expositions of theory should provide for rather light reading.

We invite you to consider using experimental methods while studying for other courses alongside your studies of experimental mathematics. Be warned, however, that such approaches may yield shortcuts that disturb the original purpose of a traditional exercise. While such examples provide excellent motivation for the study of experimental mathematics, by showcasing the way experiments can be used to gain insight, they may not give you the training in traditional mathematical methods that you would have gotten by solving such exercises by traditional means. Sometimes, experimental mathematics by computer-based computation is just *too* efficient.

For the Teacher

Like the authors, you are very likely a largely self-taught experimental mathematician yourself, and probably embark on teaching a course on experimental mathematics with some hesitation. Teaching a course in experimental mathematics is obviously very different from teaching a standard upper-level theoretical course, and you may find yourself wondering how to fill the lectures and exercise sessions when there are (almost) no theorems to prove.

In spite of the nonstandard subject matter in this book, we have found that traditional lectures over the general descriptions of the experimental modus operandi combined with selected aspects of relevant mathematical theory and discussions of some of the worked examples contained in the book combine well to keep the students interested and their learning process organized. In our experience, the essential key to a successful course in experimental mathematics is to get the students involved in the design, execution, and evaluation of small experiments as early and as often as possible. In each chapter, we include exercises of varying length and difficulty that can be used for this purpose.

Depending on the students' technical background, they may need assistance to digest the more technical chapters in the book. We have found that this need is hard to address through lectures, but is effectively handled by providing easy access to technical consultations (say, using a teaching assistant with the appropriate technical qualifications).

In the courses we have taught, students have always reacted very positively when presented with examples and exercises based on our own research. In this book, we have tried to provide a diverse collection of examples and exercises, many of which are rooted in the experimental mathematics literature rather than our experiments. We warmly recommend that you involve examples and exercises inspired by your own research in addition to the ones presented here.

In our experience, students that have completed a course in experimental mathematics based on this book are fully capable of tackling open research problems experimentally. Indeed, a major motivation for many of our students has been the promise that they would be allowed to try their hands at open problems as a part of the course.

About Maple

Throughout the book, Waterloo Maple® is used to write the computer programs needed in experimental mathematics. The book is targeted at mathematicians with no prior programming experience, and to make it accessible to this audience, we have included an introduction to basic programming in Maple. However, this is not intended to be a book on computer programming.

To make the book useful to students without much programming experience, we have found it necessary to focus on a single programming language. We chose Maple because it contains all the tools we need and because it is already in use as a computer algebra system in many universities.

Code examples are given using a notation matching the classic Maple input in Worksheet Mode rather than the 2d-mathematics notation of Document

Mode. This choice was made to make sure that it is always clear to the reader what to type into Maple to reproduce the given results. While pretty, the formatting of Document Mode will sometimes obscure the text that actually has to be input in order to reproduce the 2d-mathematics notation. This is most clearly seen when working with indices of sequences and related data structures. Document Mode's 2d input, on the other hand, has the benefit of providing useful syntax highlighting for control structures and other commands, and we leave it to the readers to decide their personal preferences. The examples given should work equally well copied into either type of Maple input. The Maple code is also available on the website of this book.

The output shown in the book has been produced with Maple 2015 (beautified for legibility in a few cases), but any recent version of Maple, say Maple 15 onwards, will support the examples and serve as a vessel for the experiments suggested throughout.

The Contents of This Book

An introduction of the basic methodology of experimental mathematics is given in Chapter 1. Focus is on the use of experimental mathematics in the development of mathematical conjectures and on the special role that counterexamples play in the experimental investigation of hypotheses. The chapter concludes with a collection of case studies, showcasing the application of experimental mathematics to a variety of mathematical problems. Some of these examples are of a historical nature, while others have been developed specifically for this book. Most of them will be revisited in later chapters and examined more carefully with the tools introduced there.

Chapter 2 contains an introduction to basic programming in Maple, laying the foundation needed for the programs discussed in the rest of the book. The topics covered include variables, procedures, control structures, and debugging. Particular focus is given to the development and use of procedures for the automated testing of hypotheses. The goal of the chapter is to develop the necessary programming skills, and the examples are mainly technical in nature. The exercises, however, give students ample opportunity to apply the programming skills they have acquired to genuine mathematical experiments. Readers already familiar with programming in Maple can skip this chapter, but not its exercises.

One of the great benefits of using computers in experimental mathematics is their ability to generate and investigate extremely large collections of data. To do this efficiently requires programming techniques involving iteration and recursion. Such techniques are presented in Chapter 3 and applied to a collection of mathematical experiments. In the case of recursion, it is shown how Maple's built-in tools can be used to drastically speed up computations.

Finally, the chapter contains a discussion of how much experimental evidence you need before believing sufficiently in a hypothesis to invest your time in the search for a proof, and we present a number of examples to show how far one may need to look to find counterexamples to a hypothesis.

As mentioned above, computers allow experimenting mathematicians to generate vast quantities of data, and in order to investigate such data systematically it must be presented in a form that is understandable and manageable to the human investigator. The visualization of mathematical structures and results plays a crucial role in this process, and Chapter 4 is devoted to the discussion of such tools. This includes an introduction to many of Maple's different plotting commands and a discussion of the construction of automated figures. Novel visualization techniques that are, for example, useful for the investigation of matrices, are investigated and applied to experimental problems. Additionally, the chapter contains a discussion of data transformations and the use of both linear and nonlinear fitting in the extraction of information from data.

Generating and visualizing data is one thing, but the real power of experimental mathematics comes from the tools that allow mathematicians to detect patterns in the investigated data, for example by recognizing the first terms of a sequence or the digits of a well-known mathematical constant like π. We call this process *symbolic inversion*, and Chapter 5 presents a collection of tools that help the experimenting mathematician detect such connections. The chapter is split into two main parts dealing with sequences and floating point numbers, respectively. Sequences are investigated using transformations, generating functions, and the *Online encyclopedia of integer sequences*. For floating point numbers, it is shown how to search for patterns using, for example, continued fractions and the powerful PSLQ algorithm. The chapter also contains a discussion of some of the fascinating *mathematical* results behind these wide-ranging tools.

In some experiments, randomness (or rather pseudorandomness) can play a crucial part in avoiding biases in the construction and investigation of experimental data, and such tools are discussed in Chapter 6. To give the reader a clear understanding of the purpose and applicability of pseudorandomness, the chapter contains a discussion of the construction of pseudorandom number generators as well as an introduction to the randomization tools that are provided in Maple. The use of pseudorandomness in experiments is highlighted by a number of examples, and the application of pseudorandomness in nondeterministic algorithms is presented via an application to primality testing.

Chapter 7 concerns the challenge of balancing the desired precision with the available time and computational resources. To facilitate this, the chapter starts out with a discussion of computational complexity and O-notation before giving a series of general purpose performance tips. In many applications, there is a trade-off between time and memory consumption, and it is shown what one can do to tip this scale in order to achieve better performance. In many cases, there is also a trade-off between precision and computational resources, and in such cases it is important to know how precisely a given quantity has been calculated. To this end, it is shown how one may gauge errors using heuristic estimates or achieve stringent bounds through the use of interval arithmetic.

Finally, Chapter 8 discusses the use of linear algebra and graph theory in efficient experimental investigations. This is meant to showcase how experimental investigations into largely unknown territory may benefit from importing ideas and results from more mature mathematical subjects. Linear algebra and graph theory are by no means the only fields that can play this role, but they do show up sufficiently often to warrant special attention. In particular, it is shown how Maple can be used for linear algebra over non standard fields and rings that may play a role in experimental mathematics. Additionally, the chapter uses graphs as the foundation for a discussion of the important mathematical concepts of *isomorphism* and *equivalence* which can sometimes be used to drastically reduce the number of cases an experimental mathematician needs to consider.

EX. 1.5.1 → Throughout the book, the exposition is supported and driven by a large collection of concrete examples. Some of these case studies are revisited several times in the book, and notes in the margin are used to track such transversal connections through the text. This makes it clear whether a given example has been examined previously in the text and whether it will be discussed again later. Specifically, the margin notes shown here would signify that the current text is a continuation of something considered in Example 1.5.1 and EX. 3.4.1 ← that this subject will be discussed again in Example 3.4.1.

Scattered throughout the text, there are boxes with short descriptions of notable events in the history of experimental mathematics. These boxes are intended to provide context and interesting anecdotes relevant to the main material, but they are largely independent of the rest of the text and are generally very light reading. Every chapter concludes with a collection of miscellaneous notes relevant to the covered material and suggestions for further reading. Most citations are deferred to these sections to increase the readability of the main text.

Exercises and Projects

Each chapter contains a collection of exercises subdivided into three categories: *warmup*, *homework*, and *projects and group work*. *Warmup* exercises are meant to be fast and straightforward training exercises testing the concepts and basic tools introduced in the chapter. Most are suitable for self-testing as well as unprepared classroom discussions. *Homework* exercises are generally more difficult and time-consuming than *warmup* exercises and are meant to train the use of experimental methods introduced in the chapter. Particularly long and/or hard exercises are underlined.

The final category contains advanced experimental projects that require the use of a wide range of the ideas and tools introduced in the preceding chapters. Each project description introduces a concrete mathematical problem that can be investigated experimentally. The questions posed in each case are meant to guide the initial investigation, but as always, the experimenter should keep an open mind and pursue all interesting results. In addition to the experimental projects, this section also contains exercises that are not particularly long or hard, but require students to work in groups.

Projects generally require a lot more work than homework exercises, and some are harder than others: Underlined exercises in this category are genuine open problems where the authors do not know the answers to all questions posed, so it may well be hard or impossible to formulate satisfactory hypotheses. After all, even an exemplary experimental investigation will not reveal interesting results if there is no structure to find. This is a fundamental condition of the experimental process that students of experimental mathematics will have to face sooner or later. We hope that these open-ended projects will give the reader a chance to experience the thrill of possible discovery that comes with developing new mathematical theory.

Acknowledgements

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Finally, we wish to express our gratitude to VILLUM FONDEN for funding the Network in Experimental Mathematics which has allowed the experimental mathematics community at the University of Copenhagen to blossom and given us the opportunity to pursue goals of experimental mathematics in our own research.

Copenhagen, July 21, 2016

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