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Preface

What This Book Is About

A finite difference (FD) formula is a local approximation, typically of a derivative, and it consists of weights that can then be applied to the values of arbitrary functions. Methods based on FD approximations are ubiquitous in modern scientific computing. They were well established for solving differential equations over a century ago, when the word "computer" referred to a person with plenty of paper, pencils, and persistence. From at first amounting to a quite straightforward use of simple formulas, readily obtained from a few terms in a Taylor expansion, many specialized FD procedures and refinements have since been developed. Finite element methods evolved around 1960, and software packages based on these are nowadays widely used, especially for many engineering applications. Other offsprings include finite volume, spectral element, and discontinuous Galerkin methods. Two additional major developments began in the early 1970s. One was to push FD stencils toward increasing sizes and orders of accuracy, leading to pseudospectral (PS) methods. The other, focusing on geometric flexibility and allowing for grid-free discretizations, replaced in their derivations polynomials with radial basis functions (RBFs). From the latter have more recently evolved RBF-generated FD methods (or RBF-FD for short), offering FD-like usage, high orders of accuracy, together with total geometric flexibility and easy implementation in any number of space dimensions.

There exists already an extensive literature in the forementioned areas. However, one theme that has not yet received as much attention is the rich middle ground between low-order and extremely high-order FD-based approximation methods. Since traditional FD methods (still a workhorse for general scientific computing) are closely related also to approximations of integrals and of fractional derivatives, some such applications are also described. This book is additionally motivated by several recent developments in these latter areas. In spite of its long history, the FD topic is still a rapidly evolving one.

What This Book Is Not About

The methods described here are centered around spatially local approximations to differential operators and include also some additional contexts where FD-inspired tools are utilized. Nodes used for discretizations may be grid based or irregularly distributed – but if so only when that is motivated by physical reasons (such as irregularly shaped boundaries or a need for locally higher resolution) rather than as artifacts of any special numerical method. In particular, we do not discuss any methods related to orthogonal polynomials, where boundary node clustering is employed purely to control the polynomial Runge phenomenon. FD spin-offs (such as finite elements, finite volume, and discontinuous Galerkin) and applications to integral equations are also not described. Furthermore, this book is not a place to look for functional analysis or for elaborate error estimates.

Brief Summary of the Main Chapters

1. Introduction to FD Methods: The history of FD approximations goes back further than that of calculus. The classical definition of a derivative is in itself an example of a very simple (and quite inaccurate) FD formula. While many of its basic properties follow quite immediately from Taylor expansions, numerous additional perspectives are very helpful in appreciating the method's strengths (and weaknesses).

2. Brief Summary of PS Methods: FD approximations of increasing orders of accuracy require larger stencil sizes. The limiting case has numerous important applications, which have been extensively treated in the literature. Our present summary aims more to provide some general insights into the pros and cons of pushing up the accuracy order than to describe PS implementations and technicalities.

3. FD Approximations for Ordinary Differential Equations (ODEs): The most common reason for wanting to approximate derivatives is to apply these to the solution of differential equations. In the case of ODEs, many of the well-established procedures are immediately related to

FD approximations – often more closely than may be apparent from how these are customarily described.

4. **Grid-based FD Approximations for Partial Differential Equations:** Although a variety of PDE solvers have been developed for different applications, quite straightforward FD-based approximations remain of great utility and importance. As for ODEs, high orders of accuracy often significantly increase computational efficiency.
5. **Mesh-Free FD Approximations:** In all the cases above, the core concept behind the FD approximations has been Taylor expansions. These are easy to work with and are in some sense optimal in their representations of functions locally around a single point. However, polynomial-based approximations in more than one dimension encounter severe difficulties if the points that approximations are based on are not regularly placed (grid based). Difficulties in solving differential equations often come from boundaries that may be irregularly shaped and from mixtures of scales that may require spatially variable resolution. It transpires that RBFs can replace (or supplement) polynomials in such situations, again leading to highly effective and accurate FD-type approximations.
6. **FD in the Complex Plane:** Measurable physical quantities do not involve complex numbers.[1] However, with most standard and special functions in the applied sciences being *analytic functions*, both mathematical analysis and computational procedures can benefit greatly from exploiting this feature. While such mathematical tools have seen much use during the last couple of centuries, the realization is far more recent that FD methods in the complex plane can also be remarkably effective.
7. **FD-based Methods for Quadrature and Infinite Sums:** This is again an area where commonly used methods on equispaced grids (the setting in which data is often available if not created just for the purpose of quadrature) relate closely to FD approximations. Complex plane FD approximations can be used for highly accurate contour integration of analytic functions.
8. **Fractional-Order Derivatives:** Although their history is nearly as long as that of regular (integer-order) derivatives, their range of applications has increased dramatically in recent decades. High-order accurate FD methods for their approximation amount to a recent development.

The main chapters are followed by seven appendices with supporting back-

[1] unless possibly in the context of quantum mechanics.

ground materials, also focused on heuristic insights and application practicalities.

Audience for Whom the Book Is Written

This book is primarily aimed toward students and researchers who are interested or actively engaged in scientific computing. For most of the material, no more background is needed than basic calculus and some knowledge of numerical analysis, linear algebra, and complex variables. This book is not intended as a sole textbook for an introductory numerical analysis or numerical differential equations course, but more for a graduate course aimed at providing the supplementary insights and perspectives that are essential for a good understanding, but which too often fall in the cracks between traditional course materials. This book will also provide educators with additional perspectives to those focused on in many textbooks.

Some General Remarks

Books with extensive mathematical content need to find a balanced path between rigor and heuristics. We tilt here quite strongly in favor of the latter, as this much more closely reflects how actual scientific computing is designed and carried out. The goal has been to present the relevant materials, not in some form of cookbook fashion, but instead to highlight the essential concepts behind different cost-effective FD-type computational opportunities. Another aspect for which a balanced path needs to be found is how much background material to include – that is, between presenting in a too terse fashion versus bloating the manuscript with topics that many readers may find unnecessary. In this regard, we tilt somewhat toward the former. In some cases, we only alert readers to computational opportunities, leaving details to cited references and to the appendices.

When developing a numerical solution strategy and a code for an application, it is often practical to start with low-order approximations, to most easily "get into the business." It will then often transpire that higher computational efficiency is needed, calling for the second step of upgrading to higher-order accurate approximations. A goal for this book is to provide perspectives for this second step.

Acknowledgments: My personal interest in the topics described in this book evolved from my PhD work at Uppsala University, supervised by Professor Heinz-Otto Kreiss. Part of my thesis was concerned with how the materials here in Chapter 1 lead toward those in Chapter 2 (i.e., how increasing-order accurate FD methods give rise to PS methods). For past professional influences and inspirations, I want also to acknowledge Professors Herbert B. Keller, Robert D. Richtmyer, Philip G. Saffman, and Gerald B. Whitham. I also thank Professor Nick Trefethen for enthusiastically reading and commenting on an early draft of this book. Most importantly, I thank my wife, Dr. Natasha Flyer, for all her love, support, and encouragement.

Software used: The manuscript was prepared in LyX (a front-end system to LaTeX).[2] The graphics and the computational results have mostly been obtained using MATLAB,[3] in some cases supplemented by the Advanpix[4] extended precision toolbox. In a few cases, brief Mathematica[5] codes have been included.

[2] LyX – The Document Processor, www.lyx.org/.
[3] MathWorks Inc., Natick, Massachusetts: www.mathworks.com.
[4] Multiprecision Computing Toolbox, Advanpix LLC, Yokohama, Japan, www.advanpix.com/.
[5] Wolfram Research, Inc., Champaign, IL.