Numerical Methods for Special Functions

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siam® Society for Industrial and Applied Mathematics • Philadelphia

10 9 8 7 6 5 4 3 2 1

Library of Congress Cataloging-in-Publication Data

Gil, Amparo.
Numerical methods for special functions / Amparo Gil, Javier Segura, Nico M. Temme.
p. cm.
Includes bibliographical references and index.
ISBN 978-0-898716-34-4 (alk. paper)
1. Functions, Special—Data processing. 2. Numerical analysis. 3. Asymptotic expansions. 4. Apporximation theory. I. Segura, Javier. II. Temme, N. M. III. Title.

QA351.G455 2007
518'.6–dc22

Numerical Methods for Special Functions

To our sons Alonso and Javier (A.G. & J.S.)

To my grandsons Ambrus and Fabian (N.M.T.)

Preface

Probably, the most extended (pseudo)definition of the set of functions known as "special functions" refers to those mathematical functions which are widely used in scientific and technical applications, and of which many useful properties are known. These functions are typically used in two related contexts:

1. as a way of obtaining simple closed formulas and other analytical properties of solutions of problems from pure and applied mathematics, statistics, physics, and engineering;

2. as a way of understanding the nature of the solutions of these problems, and for obtaining numerical results from the representations of the functions.

Our book is intended to provide assistance when a researcher or a student needs to get the numbers from analytical formulas containing special functions. This book should be useful for those who need to compute a function by their own means, or for those who want to know more about the numerical methods behind the available algorithms. Our main purpose is to provide a guide of available methods for computations and when to use them. Also, because of the large variety of numerical methods that are available for computing special functions, we expect that a broader "numerical audience" will be interested in many of the topics discussed (particularly in the first part of the book). Several levels of reading are possible in this book and most of the chapters start with basic principles. Examples are given to illustrate the use of the methods, pseudoalgorithms are given to describe technical details, and published algorithms for computing a selection of functions are described as practical illustrations for the basic methods of this book.

The presentation of the topics is organized in four parts: Basic Methods, Further Tools and Methods, Related Topics and Examples, and Software. The first part (Basic Methods) describes a set of methods which, in our experience, are the most popular and important ones for computing special functions. This includes convergent and divergent series, Chebyshev expansions, linear recurrence relations, and quadrature methods. These basic chapters are mostly self-contained and start from first principles. We expect that many of the contents are appropriate for advanced numerical analysis courses (parts of the chapters are in fact based on classroom notes); however, because the main focus is on special functions, detailed examples of application are also provided.

The second part of the book (Further Tools and Methods) contains a set of important methods for computing special functions which, however, are probably not so well known as the basic methods (at least for readers who are not very familiar with special functions).

Certainly, this does not mean that these tools are less effective than the selected basic methods; for example, the performance of uniform asymptotic expansions is quite impressive in many instances. The chapters in this second part are: Continued Fractions, Computation of the Zeros of Special Functions, Uniform Asymptotic Expansions, and Other Methods (Padé approximations, sequence transformations, best rational approximations, Taylor's method for ordinary differential equations, and further quadrature methods including the Clenshaw–Curtis and Filon methods).

The third part (Related Topics and Examples) describes some methods that are specific to certain functions. A first chapter is devoted to the (asymptotic) numerical inversion of a class of distribution functions with details for gamma and beta distributions (a topic which researchers in statistics, probability, and econometrics may find useful). A second chapter (Further Examples) describes varied topics such as the Euler summation formula (and applications), the computation of symmetric elliptic integrals (Carlson's method), and the numerical inversion of Laplace transforms.

We thank NIST for the permission to quote part of a section in the DLMF project (from the chapter "Numerical Methods") on solving ordinary differential equations by using Taylor series (our §9.5), and Frank Olver for his assistance in writing this part. We thank the SIAM editorial staff, in particular Louis Primus, for their patience and splendid cooperation.

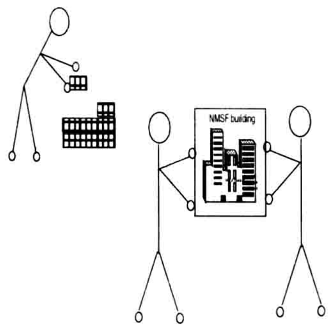
Finally, the fourth part illustrates the use of the methods by providing descriptions of specific algorithms for computing selected functions: Airy functions, Legendre functions, and parabolic cylinder functions, among others. The corresponding Fortran 90 routines can be downloaded from

http://functions.unican.es.

The web page will hold successive actualizations and extensions of the available software.

We would like to thank Dr. Van Snyder for his extensive and useful comments, and Dr. Ernst Joachim Weniger for providing us with notes, and further useful information, on Padé approximations and sequence transformations. Finally, we thank the Spanish Ministry of Education and Science for financial support (projects MTM2004-01367, MTM2006-09050).

Contents



Chapter 1
Introduction

This book deals with numerical methods for computing special functions. This means that we describe numerical methods for computing quantities for which no general definition seems to be available. What makes a function used in applications or in pure mathematics a "special function"? This is perhaps a matter of taste. There is, however, a general practical consensus regarding which functions are special: a special function should be useful for applications and should satisfy certain special properties which allow analytical treatment.

Several centuries ago the astronomers used the trigonometric functions as their basic tools in mathematics. In recent centuries the development of wave theory introduced many other functions of higher level, and many of these functions became the classical functions with which many problems from physics and other applied sciences could be described. In pure mathematics special functions arose that played a role in number theory. Also later, some of the functions that became important in statistics and probability theory were new or related to the classical functions, in particular the gamma and beta distribution functions.

There are many books now that give collections of special functions and/or describe their properties. A classical reference is the *Handbook of Mathematical Functions*, edited by Milton Abramowitz and Irene Stegun. The first edition appeared in 1964 and very soon a complete revision of this important reference, with many new chapters, will be published, together with a free accessible web version. Although the *Handbook* has introductory matter on computing and approximating elementary and special functions, complete algorithms or software are not given in either version of this reference work.

When the *Handbook* was published in 1964, a great number of algorithms and methods for computing special functions were already known, but in later years many new ideas were developed and became available in the form of mathematical software for computing special functions. Software libraries were constructed and several books appeared with collections of software, some of them claiming to cover all the functions considered in the *Handbook*.

In the present book we are not so formidably optimistic that we claim to describe computational methods or algorithms for all functions described in the old or new version of the *Handbook*. However, we describe methods which, according to our own experience, appear most frequently in the computation of special functions; this is so particularly in the first part of the book, devoted to power series, Chebyshev expansions, recurrence relations and continued fractions, and quadrature of integrals, but many other topics are also described in the book. Some methods are illustrated with explicit software examples in the last part of the book.

Airy functions are a good example of functions for which different techniques (convergent and divergent series, Chebyshev expansions, quadrature) can be of interest for computing the functions, depending on the range of the variable. Next we consider this set of functions, solutions of the second order differential equation $y'' - xy = 0$, as an example for introducing basic concepts to be described later to a greater extent. It should come as no surprise that we first discuss the solution of the differential equation using power series.

Convergent power series and differential equations

In many books of mathematical methods for physicists or engineers the words "special functions" appear for the first time when solving certain differential equations (for instance, when solving the Schrödinger equation by separation of variables) and, particularly, when trying to solve the equations by power series. Equations such as the Hermite or Bessel equations appear, which can be solved by using convergent power series.

The fact that we can find a convergent series for a specific solution of a second order ordinary differential equation may seem to indicate that the computation of such a function is of no concern. However, this is not true from a numerical point of view, even when the series does converge for any real or complex value of the argument. It could only be true if we had at our disposal a computer equipped with infinite precision arithmetic, that was infinitely fast, and that was without limitations in the numbers which can be stored. Because this ideal machine does not exist, the use of series will be limited by these three factors (as any other method).

Take, for instance, the elementary example $y'' - y = 0$, with $y_1(z) = e^z$ and $y_2(z) = e^{-z}$ as two independent solutions. Maclaurin series for y_1 and y_2 are convergent for all z. However, when $\Re z > 0$ the range of accurate computation of $y_2(z)$ should be restricted to small $|z|$, because for large $|z|$, the first terms of the series are much larger in modulus than the whole sum, leading to numerical cancellation and severe loss of significant digits. Also, the series for $y_1(z)$ is dangerous for large z because many terms need to be added. Maclaurin series should not be used very far from $z = 0$.

For not-so-elementary functions, the same types of limitations occur when using series (Chapter 2). Take for instance the very important case of the Airy functions, which are solutions of the second order ordinary differential equation

$$y''(z) - zy(z) = 0. \tag{1.1}$$

We can try power series to find the general solution. Substituting $y(z) = \sum_{n=0}^{\infty} a_n z^n$ we readily see that $a_{2+3n} = 0$, $n \in \mathbb{N}$, and that two linearly independent solutions are

$$y_1(z) = \sum_{k=0}^{\infty} 3^k \left(\frac{1}{3}\right)_k \frac{z^{3k}}{(3k)!}, \quad y_2(z) = \sum_{k=0}^{\infty} 3^k \left(\frac{2}{3}\right)_k \frac{z^{3k+1}}{(3k+1)!}, \tag{1.2}$$

where $(\alpha)_0 = 1$, $(\alpha)_k = \alpha(\alpha+1)\cdots(\alpha+k-1)$, $k \geq 1$. Elementary methods (the ratio test) can be used to prove that both series are convergent for any complex value of z.

At this moment, let us restrict the problem to real positive $z = x$. We observe that both $y_1(x)$ and $y_2(x)$ are positive and increasing for $x > 0$; all the terms of the series are positive and no cancellations occur. Now, because all the solutions of the differential equation can be written as $y(x) = \alpha y_1(x) + \beta y_2(x)$, and both $y_1(x)$ and $y_2(x)$ tend to $+\infty$ as $x \to \infty$, the equation necessarily has a solution $f(x)$, called a *recessive solution*, such that $f(x)/y(x) \to 0$ for any other solution $y(x)$ not proportional to $f(x)$.

Indeed, as $x \to +\infty$, either $y_1(x)/y_2(x) \to 0$, giving that $y_1(x)$ is recessive, or $y_2(x)/y_1(x) \to 0$, giving that $y_2(x)$ is recessive, or $y_1(x)/y_2(x) \to C \neq 0$, giving that $y_1(x) - Cy_2(x)$ is recessive. The last possibility is what happens for the recessive solutions of (1.1), with $C = 3^{1/3}\Gamma(2/3)/\Gamma(1/3)$. Again, for an algorithm the Maclaurin series can only be considered for not too large x, particularly for computing the recessive solution (such as for e^{-x} in the former example).

Later we will see that the recessive solution is a multiple of $\mathrm{Ai}(z)$, which is exponentially small at $+\infty$, and both $y_1(z)$ and $y_2(z)$ given in (1.2) are exponentially large. Hence, the solutions $y_1(z)$ and $y_2(z)$ cannot be used to compute all solutions of (1.1) for all values of z, in particular when z is large, because this may introduce large errors. We say that $y_1(z)$ and $y_2(z)$ do not constitute a *numerically satisfactory pair of solutions* of (1.1) at $+\infty$, because the recessive solution cannot be computed by these two for large positive z. The same situation occurs when considering differential equations for other special functions. For a graph of the Airy function $\mathrm{Ai}(x)$, see Figure 1.1.

Obviously, one should never compute an exponentially decreasing function for large values of the variable as a linear combination of two increasing functions for values of the argument for which the computed value is much smaller than the increasing functions. Subtracting two large quantities for obtaining a small quantity is a numerical disaster. For the recessive Airy function $\mathrm{Ai}(x)$ we have $\mathrm{Ai}(1) = 0.135\ldots$, and the loss of significant digits becomes noticeable when we use the functions of (1.2) when $x \geq 1$. Therefore, if we need to compute the recessive solution, we must consider an independent method of computation for this function.

In addition, one needs to pay attention to different ranges of the variable in order to select a numerical satisfactory pair. For instance, going back to the elementary case, $y'' - y = 0$, the solutions $y_1(z) = e^z$ and $y_2(z) = e^{-z}$, which constitute a numerically satisfactory pair when $\Re z \gg 0$, but this pair is not a satisfactory pair near $z = 0$. Near the origin, it is better to include $y_3(z) = \sinh z = (y_1(z) - y_2(z))/2$ as a solution when $|z|$ is small; a companion solution could be $y_4(z) = \cosh z$. Of course, $y_3(z)$ and $y_4(z)$ do not constitute a numerically satisfactory pair when $|\Re z|$ is large.

Liouville–Green approximation and dominant asymptotic behavior

More information on the behavior of the solutions of a linear second order differential equation can be obtained by transforming the equation. It is a straightforward matter to check (see also §2.2.4) that, if $y(z)$ is a solution of (1.1), then the function $Y(z) = z^{1/4}y(z)$ satisfies the equation

$$\ddot{Y}(\zeta) + \left(-1 + \frac{5}{36\zeta^2}\right) Y(\zeta) = 0 \tag{1.3}$$

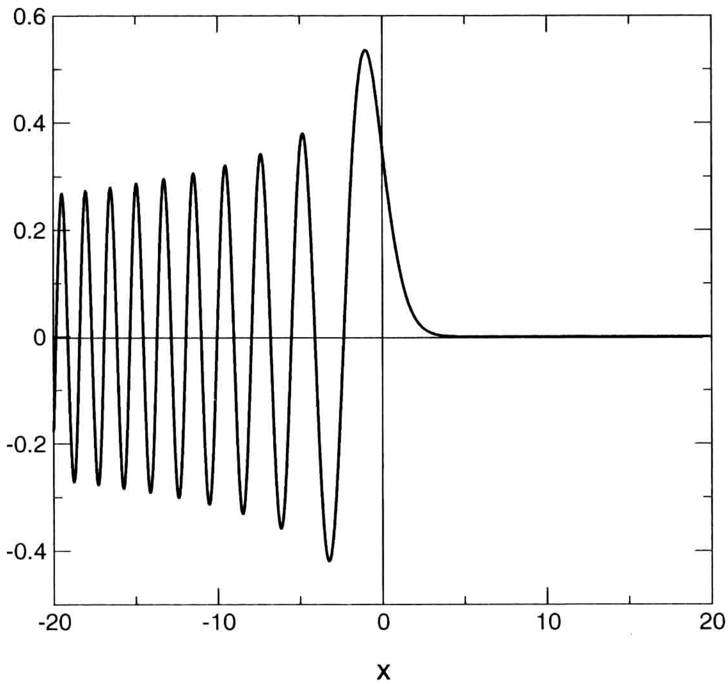


Figure 1.1. *The Airy function* Ai(x) *is oscillating for* $x < 0$ *and exponentially small for* $x \to +\infty$.

in the variable $\zeta = \frac{2}{3}z^{3/2}$. Looking at (1.3), we can expect that for large ζ the term $5/(36\zeta^2)$ will be negligible and that the solutions will behave exponentially, $Y(\zeta) \sim \exp(\pm\zeta)$. Undoing the changes, we expect that the recessive solution of (1.1) behaves as $z^{-1/4}\exp(-\frac{2}{3}z^{3/2})$. A more detailed analysis [168, Chap. 6] shows that this approximation (the Liouville–Green approximation) makes sense. Therefore, we are certain that a recessive solution exists which decreases exponentially.

Condition of solution of ordinary differential equations

It is not a surprise that the recessive solutions of the defining differential equations are usually the most important in applications; indeed, physical quantities are by nature finite quantities and functions representing these quantities should be bounded. From a numerical point of view, as explained, a special treatment for these functions is needed.

Anyway, isn't the Airy function a solution of a second order differential equation? Isn't it true that most students who have received a course on numerical analysis are familiar with methods for solving second order differential equations? Isn't it true that numerical methods for second order differential equations apply to any solution of the equation? So, can we rely blindly on, let's say, Runge–Kutta? Or do we need more analysis? The answer is, obviously, yes, analysis is necessary and one needs to know if the desired solution is recessive.