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Recent software developments for special functions in the Santander–Amsterdam project

Amparo Gil [a], Javier Segura [b,*], Nico M. Temme [c]

[a] Departamento de Matemática Aplicada y Ciencias de la Computación, ETSI Caminos, Universidad de Cantabria, 39005 Santander, Spain
[b] Departamento de Matemáticas, Estadística y Computación, Univ. de Cantabria, 39005 Santander, Spain
[c] IAA, 1391 VD 18, Abcoude, The Netherlands [1]

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ABSTRACT

We give an overview of published algorithms by our group and of current activities and future plans. In particular, we give details on methods for computing special functions and discuss in detail two current lines of research. Firstly, we describe the recent developments for the computation of central and non-central χ-square cumulative distributions (also called Marcum Q-functions), and we present a new quadrature method for computing them. Secondly, we describe the fourth-order methods for computing zeros of special functions recently developed, and we provide an explicit example for the computation of complex zeros of Bessel functions. We end with an overview of published software by our group for computing special functions.

1. Introduction

Our project on software developments for special functions started in 1997. Earlier we published a number of papers in this area, and the plan was to combine all our expertise in order to produce quality software based on a selection of the many methods available for special functions, and by justifying these methods in particular cases with the help of elements of numerical and mathematical analysis, such as recurrence relations, numerical quadrature and asymptotic expansions.

We discuss current activities in two different lines of research. Firstly, we discuss the computation of χ-square cumulative distributions and, in particular, we present a new quadrature method for computing the non-central distribution, also called Marcum's Q-function. Secondly, we describe in a unified way two recent methods for computing zeros of special functions (for real and complex zeros), we give an explicit example of computation for complex zeros of Bessel functions and discuss plans for software implementations. We end with an overview of our published software for computing special functions.

First, we briefly outline the basic methods and principles we consider in the construction of special function software.

2. Numerical methods and basic principles

Our book [33] "Numerical methods for special functions" appeared in 2007 and describes four basic methods that we have used in writing software. These methods are: convergent and asymptotic series, Chebyshev expansions, linear recurrence relations and quadrature methods. The book also describes numerical methods for computing continued fractions,

* Corresponding author.
E-mail addresses: amparo.gil@unican.es (A. Gil), javier.segura@unican.es (J. Segura), Nico.Temme@cwi.nl (N.M. Temme).
[1] Former address: CWI, Science Park 123, 1098 XG Amsterdam, The Netherlands.

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methods for computing zeros of special functions and the computation with uniform asymptotic expansions, among other topics. Usually, several of these methods have to be combined for computing a special function.

2.1. Our principles of designing algorithms

Our approach in making software can be described by the following principles.

1. The main objective is to develop Fortran 90 codes which produce reliable double precision values. We use Maple or Mathematica for obtaining coefficients in expansions and for verifying algorithms, but not usually in the final product. The exceptions are some codes for computing zeros of special functions.
2. A given special function is usually a special case of a more general function. Our approach is bottom-up and when a simple but important function is demanding software, we prefer to start with the "simple" case. For example: Airy functions are special cases of the more general Bessel functions, but we have written codes for the Airy functions themselves.
3. We accept that it is necessary to combine several methods in order to compute a function accurately and efficiently for a wide range of its variables.
4. We accept that a theoretical error analysis is usually impossible for functions with several real or complex variables. We accept more empirical approaches.
5. The accuracy analysis is usually done by using functional relations, such as Wronskian relations or by comparing with an alternative method of computation.
6. The selection of methods in different parameter domains is based on speed and accuracy, where the latter may prevail. For large real or complex parameters scaling of the result is useful to avoid underflow or overflow in our finite arithmetic environment.

3. Incomplete gamma functions, Marcum Q-function

As before commented, present interest is focused on distribution functions, in particular on the incomplete gamma functions (see [38]) and generalizations. Incomplete gamma functions are the central χ-square cumulative distributions and are defined by

$$\gamma(a,x)=\int_0^x t^{a-1}e^{-t}\,dt, \qquad \Gamma(a,x)=\int_x^\infty t^{a-1}e^{-t}\,dt. \tag{3.1}$$

We concentrate on the ratios

$$P(a,x)=\frac{1}{\Gamma(a)}\gamma(a,x), \qquad Q(a,x)=\frac{1}{\Gamma(a)}\Gamma(a,x), \tag{3.2}$$

where we assume that a and x are positive. We can use the well-known series expansions, asymptotic expansions, recurrence relations, and a method based on the uniform asymptotic representation of these ratios in terms of the complementary error function. Apart from the last method, we mainly use the methods considered in [14,15], although Gautschi used a different set of functions and also negative values of a. For applications in mathematical statistics and probability theory the ratios in (3.2) are more relevant. Furthermore, in [38] we described algorithms for inverting the incomplete gamma ratios, and the algorithm improves the one given in [8,9].

The results of the algorithms for the incomplete gamma ratios are used in our current project on the generalized Marcum Q-function, which is defined in (3.5) and (3.6). A paper with full details of our numerical computations has been submitted [40]. The relation with the incomplete gamma functions becomes clear when expanding the Bessel function in its power series, which gives

$$Q_\mu(x,y)=e^{-x}\sum_{n=0}^\infty \frac{x^n}{n!}Q(\mu+n,y), \tag{3.3}$$

and

$$P_\mu(x,y)=e^{-x}\sum_{n=0}^\infty \frac{x^n}{n!}P(\mu+n,y). \tag{3.4}$$

3.1. A new quadrature method for computing the Marcum Q-function

As we have explained in [33, Ch. 5], numerical quadrature can be an important tool for evaluating special functions. In particular, when selecting suitable integral representations for these functions. In Chapter 12 of our book we have given