Algorithm 969: Computation of the Incomplete Gamma Function for Negative Values of the Argument

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An algorithm for computing the incomplete gamma function $\gamma^*(a, z)$ for real values of the parameter a and negative real values of the argument z is presented. The algorithm combines the use of series expansions, Poincaré-type expansions, uniform asymptotic expansions, and recurrence relations, depending on the parameter region. A relative accuracy $\sim 10^{-13}$ in the parameter region $(a, z) \in [-500, 500] \times [-500, 0)$ can be obtained when computing the function $\gamma^*(a, z)$ with the Fortran 90 module **IncgamNEG** implementing the algorithm.

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1. INTRODUCTION

The incomplete gamma function $\gamma^*(a, z)$ is defined by

$$\gamma^*(a, z) = \frac{z^{-a}}{\Gamma(a)}\gamma(a, z) = \frac{1}{\Gamma(a)}\int_0^1 t^{a-1}e^{-zt}dt, \tag{1}$$

where $\gamma(a, z)$ is the lower incomplete gamma function [Paris 2010, Equation (8.2.1)].

The function $\gamma^*(a, z)$ is real for positive and negative values of a and z.

Incomplete gamma functions appear in a large number of scientific applications. For positive values of z, they are related to the central gamma and chi-squared distribution

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functions (positive a) and to exponential integrals (negative a). There are numerous application areas for positive z, as, for example, in Krishnamoorthy [2006] and Collins [1989]. Algorithms and software are available for this parameter region [Gautschi 1979; Didonato and Morris 1986; Gil et al. 2012]. For negative z, the incomplete gamma functions appear, for instance, in the study of Bose plasmas [Kowalenko and Frankel 1994; Kowalenko 1998] and in the analysis of the Helmholtz equation [Moroz 2006; Linton 2010]. However, unlike the positive z case, software to support this case is very limited. Only recently has an algorithm been constructed for negative z [Thompson 2012], and this is restricted for half-integer values of a.

In this article, we describe an algorithm for computing the function $\gamma^*(a, z)$ for a real and $z < 0$. Our algorithm improves the range of computation of Thompson [2012] by allowing real values of a. The computational methods used in our algorithm are as follows:

(a) series expansions, recurrence relations, and uniform asymptotic expansions for $a < 0$;
(b) series expansions and Poincaré-type expansions [Olver 1997, p. 16] for $a > 0$.

A Fortran 90 module implementing the algorithm is provided. Numerical tests show that the relative accuracy is close to 10^{-13} in the parameter region $(a, z) \in [-500,\ 500] \times [-500,\ 0)$. This module complements a previous algorithm for the incomplete gamma function for positive values of the parameters [Gil et al. 2012].

2. METHODS OF COMPUTATION

We describe the methods of computation used in the algorithm and in the numerical tests. Details on the region of application of each method are discussed in Section 4.

2.1. Recurrence Relations

Recurrence relations are useful methods of computation when initial values are available for starting the recursive process. Also, recurrence relations can be used for testing the function values obtained by alternative methods. Usually, the direction of application of the recursion cannot be chosen arbitrarily, and the conditioning of the computation of a given solution fixes the direction.

The function $\gamma^*(a, z)$ satisfies the following inhomogeneous recursion [Paris 2010, Equation (8.8.4)]:

$$z\gamma^*(a+1, z) = \gamma^*(a, z) - \frac{e^{-z}}{\Gamma(a+1)}. \tag{2}$$

When both a and z have negative values, replacing $(a,\ z)$ by $(-a-1,\ -z)$ and using the reflection formula $\Gamma(a+1)\Gamma(-a) = -\frac{\pi}{\sin(\pi a)}$ in Equation (2), we obtain [Temme 1996, Equation (4.1)]

$$\gamma^*(-a-1, -z) + z\gamma^*(-a, -z) = -\frac{1}{\pi}\sin(\pi a)e^z\Gamma(a+1). \tag{3}$$

We may also combine two first-order recursions of Equation (2) to obtain the three-term homogeneous recurrence relation

$$z(a+1)\gamma^*(a+2, z) - (a+1+z)\gamma^*(a+1, z) + \gamma^*(a, z) = 0. \tag{4}$$

Starting from Equation (3), we obtain

$$\gamma^*(-a-2, -z) + (z+a+1)\gamma^*(-a-1, -z) + z(a+1)\gamma^*(-a, -z) = 0. \tag{5}$$

An advantage of using the relation in Equation (5) is that possible accuracy problems in the computation of the inhomogeneous term in Equation (2) or Equation (3) are avoided.

2.2. Series Expansion

A series expansion for $\gamma^*(a,z)$ is given by Paris [2010, Equation (8.7.1)]

$$\gamma^*(a,z)=\frac{1}{\Gamma(a)}\sum_{k=0}^{\infty}\frac{(-z)^k}{k!(a+k)}\,. \tag{6}$$

As pointed out in Bailey and Borwein [2015] and discussed later (see Section 3), this series proves to be very useful computationally. In this form, the series cannot be applied when $a=-n,\ n=1,2,\ldots,$ and special care needs to be exercised when $a=-n+\epsilon$ and ϵ is small. In this case, it is convenient to rewrite the series as

$$\gamma^*(-n+\epsilon,z)=z^n\frac{\Gamma(1+n-\epsilon)}{n!}\frac{\sin\pi\epsilon}{\pi\epsilon}+\frac{1}{\Gamma(-n+\epsilon)}\sum_{k=0,k\neq n}^{\infty}\frac{(-z)^k}{k!(-n+\epsilon+k)}\,. \tag{7}$$

Using Equation (7), the series can be computed as $\epsilon\to 0$ and we obtain, in the limit, the result [Paris 2010, Equation (8.4.12)]

$$\gamma^*(-n,z)=z^n. \tag{8}$$

2.3. Uniform Asymptotic Expansion for $a<0$

When a and z have large negative values, it is convenient to use the uniform asymptotic expansion described in Temme [1996], where the error function is used as a main approximant. Replacing $(a,\ z)$ with $(-a,\ -z)$, we have

$$\gamma^*(-a,-z)=z^a\left\{\cos(\pi a)-\sqrt{\frac{2a}{\pi}}e^{\frac{1}{2}a\eta^2}\sin(\pi a)\left[\sqrt{\frac{2}{a}}F\left(\eta\sqrt{\frac{a}{2}}\right)+\frac{1}{a}T_a(\eta)\right]\right\}, \tag{9}$$

where η is defined by

$$\frac{1}{2}\eta^2=\lambda-1-\log(\lambda),\quad \lambda=\frac{z}{a},\quad \operatorname{sign}(\eta)=\operatorname{sign}(\lambda-1). \tag{10}$$

The choice of the sign is based on the similarity of the graphs of the η-function (a parabola) and of the λ-function (a convex function for $\lambda>0$, with its zero-minimum at $\lambda=1$, and with the shape of a parabola).

As noted in Temme [1996], it is also useful to consider the normalized function $\widetilde{\gamma}_a(z)$ defined by the relation

$$\gamma^*(-a,-z)=z^a\cos(\pi a)+\sin(\pi a)\Gamma(a)e^z\widetilde{\gamma}_a(z), \tag{11}$$

giving

$$\widetilde{\gamma}_a(z)=-\frac{a}{\pi\Gamma^*(a)}\left[\sqrt{\frac{2}{a}}F\left(\eta\sqrt{\frac{2}{a}}\right)+\frac{1}{a}T_a(\eta)\right]. \tag{12}$$

Using Equation (11) in the inhomogeneous recursion, Equation (3), we obtain

$$-\widetilde{\gamma}_{a+1}(z)+\frac{z}{a}\widetilde{\gamma}_a(z)+\frac{1}{\pi}=0. \tag{13}$$

In Equations (9) and (12), $F(z)$ is Dawson's integral,

$$F(z)=e^{-z^2}\int_0^z e^{t^2}dt=-\frac{1}{2}i\sqrt{\pi}e^{-z^2}\operatorname{erf} iz,$$

where erf is the error function.

Dawson's integral can be computed using a continued fraction representation. In our algorithm, we use the representation given in Cuyt et al. [2008, Equation (13.1.13b)]. This continued fraction works very well for small and large values of z.

The function $T_a(\eta)$ in Equations (9) and (12) has an asymptotic expansion in negative powers of a,

$$T_a(\eta) \sim \sum_{n=0}^{\infty} (-1)^n \frac{C_n(\eta)}{a^n}, \tag{14}$$

where the coefficients $C_n(\eta)$ may be obtained starting from the differential equation satisfied by $T_a(\eta)$:

$$\frac{d}{d\eta} T_a(\eta) + a\eta T_a(\eta) = a(f(\eta)\Gamma^*(a) - 1), \tag{15}$$

with $f(\eta)$ and $\Gamma^*(a)$ given by

$$f(\eta) = \frac{\eta}{\lambda - 1}, \quad \Gamma^*(a) = \sqrt{a/(2\pi)} e^a a^{-a} \Gamma(a). \tag{16}$$

Substituting the asymptotic expansion (Equation (14)) into Equation (15) and using the expansion of the reciprocal gamma function

$$\frac{1}{\Gamma^*(a)} \sim \sum_{n=0}^{\infty} \frac{\gamma_n}{a^n}, \ a \longrightarrow \infty, \tag{17}$$

it is possible to find the following relations for the coefficients $C_n(\eta)$

$$C_0(\eta) = \frac{1}{\lambda - 1} - \frac{1}{\eta}, \quad \eta C_n(\eta) = \frac{d}{d\eta} C_{n-1}(\eta) + \gamma_n f(\eta), \ n \geq 1. \tag{18}$$

When $|\eta|$ is small ($\lambda \to 1$) the removable singularities in the representations of the coefficients C_n can be a source of problems in numerical computations. In Temme [1996], Maclaurin expansions for the coefficients $C_0, \ldots, C_6$ were used to generate the values given in Table 4.1 in that reference. In the present algorithm, we use a different approach. Instead of expanding each coefficient $C_n(\eta)$, we expand the function $T_a(\eta)$ of Equation (14) in powers of η:

$$T_a(\eta) = \sum_{n=0}^{\infty} \omega_n \eta^n. \tag{19}$$

To compute the coefficients ω_n, we use the differential equation for $T_a(\eta)$ given in Equation (15). Substituting the expansion (19) into Equation (15) and using the coefficients d_n in the expansion

$$\frac{\eta}{\lambda - 1} = \sum_{n=0}^{\infty} d_n \eta^n, \quad d_0 = 1, \quad d_1 = -\frac{1}{3}, \quad d_2 = \frac{1}{12}, \tag{20}$$

we obtain

$$\omega_1 = a(\Gamma^*(a) - 1), \tag{21}$$

and, for general ω_n, the recursion relation

$$\omega_n = -\frac{n+2}{a} \omega_{n+2} + d_{n+1} \Gamma^*(a), \quad n = 0, 1, 2, \ldots. \tag{22}$$

If we write

$$\omega_n = \alpha_n \Gamma^*(a), \quad n = 0, 1, 2, \ldots, \tag{23}$$

then we have the recursion

$$\alpha_n = -\frac{n+2}{a}\alpha_{n+2} + d_{n+1}, \quad n = 0, 1, 2, \ldots. \tag{24}$$

Then, we choose a positive integer N, put $\alpha_{N+2} = \alpha_{N+1} = 0$, and compute the sequence

$$\alpha_N, \alpha_{N-1}, \ldots, \alpha_1, \alpha_0 \tag{25}$$

from the recurrence relation (24).

Because (see Equations (21) and (23))

$$\frac{1}{\Gamma^*(a)} = 1 - \frac{1}{a}\alpha_1, \tag{26}$$

we have

$$T_a(\eta) \approx \frac{a}{a - \alpha_1} \sum_{n=0}^{N} \alpha_n \eta^n \tag{27}$$

as an approximation for $T_a(\eta)$.

2.4. Poincaré-Type Expansion for $a > 0$

A Poincaré-type expansion that is useful for large $|z|$ and valid for all a bounded can be obtained using the relation of $\gamma^*(a, z)$ to the Kummer function $M(a, b, z)$,

$$\gamma^*(a, z) = \frac{1}{\Gamma(a+1)} M(a, 1+a, -z), \tag{28}$$

and the expansion given in Olde Daalhuis [2010, Equation (13.7.1)].

The resulting expression is given by

$$\gamma^*(a, -z) \sim \frac{e^z}{z\Gamma(a)} \sum_{n=0}^{\infty} \frac{(1-a)_n}{z^n}. \tag{29}$$

2.5. Numerical Quadrature

For $a > 0$, it is also possible to use numerical quadrature to compute the function $\gamma^*(a, z)$. Starting from Equation (1), we replace z by $-z$,

$$\gamma^*(a, -z) = \frac{1}{\Gamma(a)} \int_0^1 y^{a-1} e^{zy} dy,$$

We can then use a quadrature rule to compute this integral to the desired accuracy. One approach is to consider a change of variable that transforms this integral into one that may be computed effectively using the trapezoidal rule. A suitable case for this is when the integrand decays as a double exponential in the real line (see Takahasi and Mori [1973/74] and Gil et al. [2007, Section 5.4]).

We can obtain such an integral representation by using the change of variables $r = \log(\frac{y}{1-y})$. Then,

$$\gamma^*(a, -z) = \frac{1}{\Gamma(a)} \int_{-\infty}^{\infty} (1 + e^{-r})^{-(a+1)} e^{z(1+e^{-r})^{-1}} e^{-r} dr, \tag{30}$$

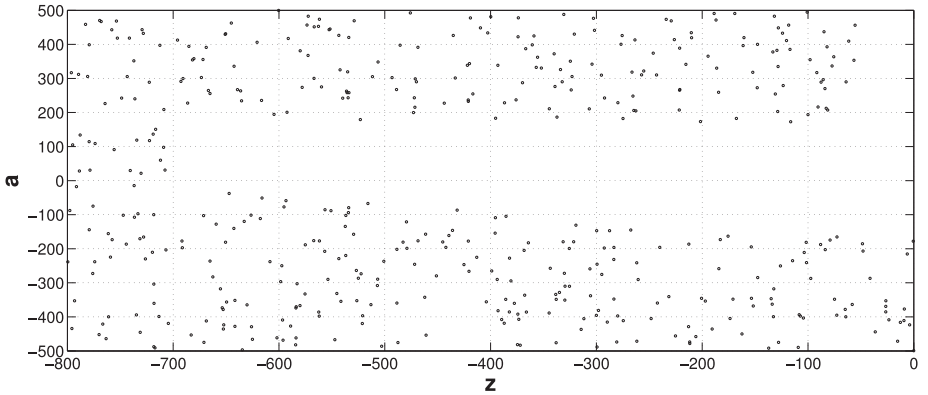

Fig. 1. Overflow/underflow limitations in double precision arithmetic in the region $(z, a) \in (-800,\ 0) \times (-500,\ 500)$ when computing the function $\gamma^*(a, z)$. The points correspond to values of the variables for which the computation either overflows or underflows.

and writing $r = \sinh(t)$, we arrive at

$$\gamma^*(a, -z) = \frac{1}{\Gamma(a)} \int_{-\infty}^{\infty} \phi(t)^{a+1} e^{z\phi(t)} e^{-r(t)} \cosh(t) dt, \tag{31}$$

where $\phi(t) = (1 + e^{-r(t)})^{-1}$.

The integrand of Equation (31) then has double exponential behaviour as $|t| \to +\infty$, which is suitable for the application of the trapezoidal rule. For numerical use, the integral should conveniently truncated by choosing only a finite interval of integration.

We note here that this quadrature approach is not used in the final version of the algorithm, as faster methods are available. However, it does provide a useful method for testing purposes.

3. NUMERICAL TESTING AND PERFORMANCE

For $a < 0$, we tested the performance of the uniform asymptotic expansion over a wide range of parameters using the normalized gamma function $\widetilde{\gamma}_a(z)$ defined in Equation (12) and the recurrence relation given in Equation (13). Using 10^8 random points over the region of the (z, a)-plane $[-1000,\ 0) \times [-1000,\ 0]$, we obtained an accuracy $\sim 10^{-14}$ in the whole region with the exception of the strips $|a| < 4.5$ and $|z| < 1.5$. The range of computation of the $\gamma^*(a, z)$ is more limited due to overflow/underflow problems in double precision arithmetic, as can be seen in Figure 1. Function values underflow (overflow) in standard IEEE double precision arithmetic for large positive (negative) values of a. For that reason, we have limited the rest of the tests to the region of the (z, a)-plane $[-500,\ 0) \times [-500,\ 500]$.

The series expansions of Section 2.2 have been tested against a Maple implementation using 30-digit accuracy for $a < 0$ in the regions $(z, a) \in [-500,\ 0) \times [-5,\ 0]$ and $(z, a) \in [-1.5,\ 0) \times [-500,\ 0]$. The maximum relative error obtained was $\sim 10^{-13}$, although a large number of terms are needed for computing the series when $|z|$ is large. In this case, a more efficient method of computation is to combine the use of recurrence relations and uniform asymptotic expansions. In particular, we compute first the normalized gamma function $\widetilde{\gamma}_{\tilde{a}}(z)$ for a value of the parameter $\tilde{a}$ within the range of validity of the uniform asymptotic expansion and then take few steps in the backward direction of the recursion (13). The function $\gamma^*(a, z)$ is finally computed using Equation (11).

As already mentioned in Section 2.2, we need to be careful in the computation when a is close to an integer, that is, $a = -n + \epsilon$, where ϵ is small. To avoid loss of accuracy both

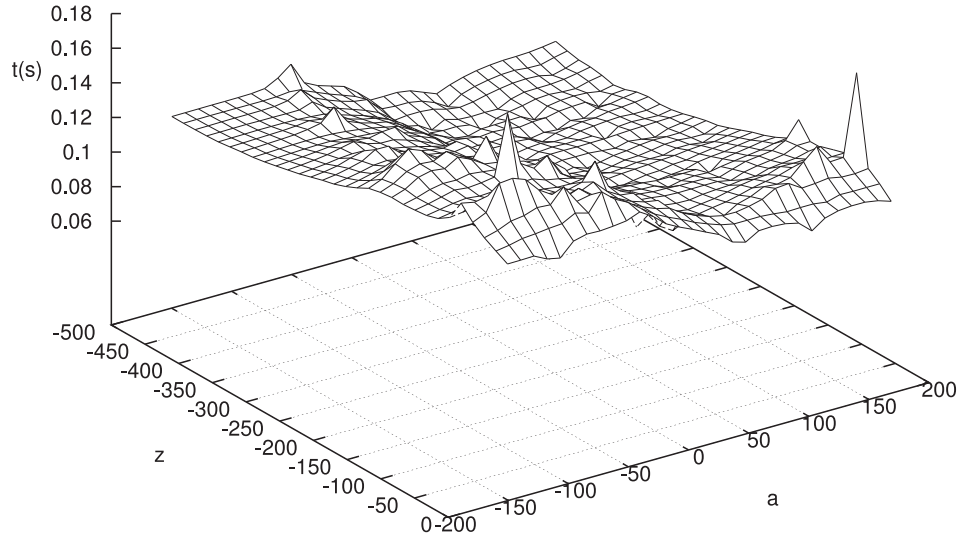

Fig. 2. CPU time spent by the algorithm as a function of the variables a and z. The times shown correspond to 50, 000 function evaluations.

in the series expansions and when computing the coefficients with the trigonometric functions in Equation (9), the input argument, a, is defined as a quadruple precision real variable in our implementation.

For a positive, testing is made by comparing the available methods of computation: series expansions (Equation (6)), numerical quadrature (Equation (31)), and Poincaré-type expansions (Eqution (29)). Accuracy close to 10^{-14} is obtained in the region $(z, a) \in [-500,\ 0) \times [0,\ 500]$ using the series expansion. Numerical quadrature is also accurate over the whole region with the exception of a-values close to zero, where there is some loss of accuracy in the computed function values. As in the case of $a < 0$, the series expansion needs a large number of terms when $|z|$ is large, which makes the use of the Poincaré-type expansion more efficient for $|z| > 50$.

Figure 2 shows the CPU time used by the Fortran version of the algorithm in evaluating the function at 50,000 values of a and z on a 2GHz Intel Core i5-43100 with Windows 7 Professional. As we can see, the times are quite uniform across the whole range.

4. COMPUTATIONAL SCHEME

From the results obtained in the previous section, we may state a stable computational scheme for evaluating the function $\gamma^*(a, z)$ as follows:

(1) For $a > 0$,
    If $z < -50$, then compute the function using the Poincaré-type expansion (29).
    Otherwise, compute using the series expansion (6).
(2) For $a < 0$,
    If $a = -n,\ n \in \mathbb{N}$, then use the expression given in Equation (8).
    Otherwise,
        If $a > -5$ or $z > -1.5$,
            If $z > -100$, then use the series expansion (6) or the expression (7) if $a = -n + \epsilon$ and ϵ is small.
            Otherwise, use the uniform asymptotic expansion (9) and the recursion relation given in Equation (13).
        Otherwise, compute the function using the uniform asymptotic expansion (9).

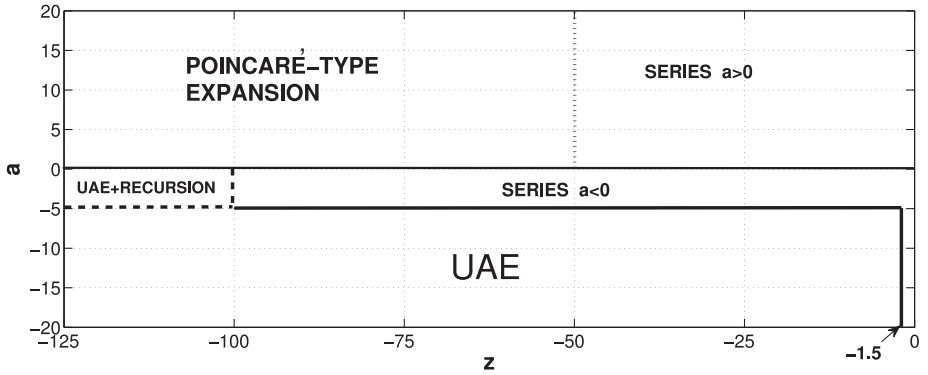

Fig. 3. Methods for computation of the $\gamma^*(a, z)$ function used in the final algorithm. UAE is the uniform asymptotic expansion of Section 2.3. The recursion relation is given in Equation (13).

The different methods of computation used in the algorithm, with the exception of the method for $a = -n$, $n \in \mathbb{N}$, are shown in Figure 3. The domains of computation are established following a compromise between efficiency and accuracy: We choose the most accurate method, and where two methods are equally accurate in a certain parameter region, we choose the fastest.

The resulting algorithm improves the range of computation of the algorithm presented in Thompson [2012]. Thompson's algorithm considers the computation of the lower incomplete gamma function for negative real values of the argument z and half-integer values of the parameter a using a function $S_n(z)$, n integer, and $z > 0$, related to the lower incomplete gamma function by $\gamma(n + 1/2, -z) = i(-1)^n e^z z^{n+1} S_n(z)$. The relation of the function $S_n(z)$ to the $\gamma^*(a, z)$ is then given by $S_n(z) = \Gamma(n + 1/2)e^{-z}\gamma^*(n + 1/2, -z)$. Precomputed values in Maple to initiate analytic continuation are used in Thompson's algorithm which, in the implementation available in Thompson [2012], seems to be restricted to z values in the interval [0, 200]. Our approach extends the range of computation to real values of the parameter a and larger negative values of the argument z, and it does not depend on values precomputed in Maple.

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