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gamma function with imaginary second
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Report TW441, January 2006



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Abstract

Even though the two term recurrence relation satisfied by the incomplete gamma function is asymptotically stable in at least one direction, for an imaginary second argument there can be a considerable loss of correct digits before stability sets in. We present an approach to compute the recurrence relation to full precision, also for small values of the arguments, when the first argument is negative and the second one is purely imaginary. Furthermore, the method we present is valid for the computation of solutions of general first order difference equations.

1 Introduction

The (upper) incomplete gamma function $\Gamma(x, y)$ is defined as [1, p. 260]

$$\Gamma(x, y) = \int_y^\infty e^{-t} t^{x-1} dt$$

where x and y are complex variables and the integration path does not cross the negative real axis. In this definition it is assumed that t^x takes its principal value and that $|\arg y| < \pi$.

Many special functions can be expressed in terms of the incomplete gamma function, e.g. the exponential integral, the error functions, Fresnel integrals and Dawson's integral. Some applications of this function are in the smooth interpretation of the Stokes phenomenon for certain integrals and special functions [2, 4, 5] and the computation of the Riemann zeta function on the critical line [6].

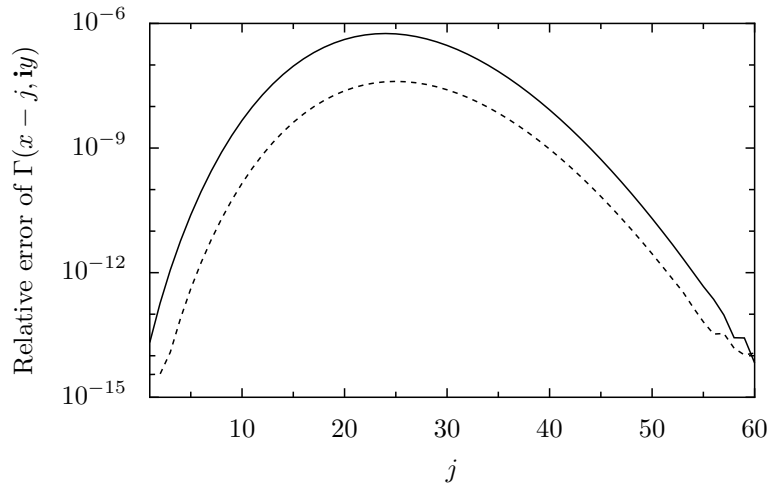


Figure 1: Error in recurrence for $\Gamma(-x - j, \mathbf{i}y)$ for $x = 1$, $j = 0, \dots, 60$ and $y = 25$. The solid line shows the relative error when the recurrence is computed starting from the value at the left and going to the right, the dashed line corresponds to going from right to left.

A recent application of this function appears in an algorithm to numerically evaluate certain integrals containing products of Bessel functions, as described in [11, 10]. This algorithm requires the evaluation of the incomplete gamma function over a large range of values of the form

$$\Gamma(-x - j, \mathbf{i}y), \quad j = 0, 1, \dots, s \quad (1)$$

where x is a positive real number, y is a real number, \mathbf{i} is the imaginary unit and s is a positive integer. It is well known that the incomplete gamma function satisfies the two term recurrence formula

$$\Gamma(x + 1, y) = x\Gamma(x, y) + y^x e^{-y}, \quad (2)$$

see e.g. [1, p. 260–262]. Using this formula, it seems that we only have to evaluate the incomplete gamma function once in (1) and can compute the other values recursively, thus seriously reducing the computational effort. However, it turns out that for the case of imaginary y , instability may occur both using forward and backward recurrence. This means that many digits are lost if we start from $\Gamma(-x, \mathbf{i}y)$ and work towards $\Gamma(-x - s, \mathbf{i}y)$, but also when we start from $\Gamma(-x - s, \mathbf{i}y)$ and go in the other direction. This is

illustrated in Figure 1, which shows the relative error on $\Gamma(-x - j, iy)$ as a function of j for $x = 1$, $y = 25$ and $s = 60$. Computations were done in double precision and the initial values were correct up to machine precision. It may be that the recurrence is *asymptotically* stable in one direction (i.e. for large j), but this is of very little use in practice.

In the next section we analyse the *relative* error propagation in general first order difference equations and discuss a simple method of computing a range of solutions without any loss of accuracy. In the rest of the paper we apply this to the specific case of the incomplete gamma function and indicate that for all values of x and y under consideration, the range (1) can be computed to full precision. The main motivation for writing this paper is that the algorithm presented here effectively improves the performance of the program in [11]. For the test set discussed in [12], the number of evaluations of the incomplete gamma function is reduced from 2027 to 177, with a reduction in time from 0.57s to 0.08s (there is some organisational overhead in the recurrence relation).

2 Relative error propagation in first order difference equations

Let us consider the difference equation

$$y_n = a_n y_{n-1} + b_n$$

where a_n and b_n are arbitrary complex parameters. If we want to compute y_n using this recurrence, starting from the value y_m with $m \leq n$, it is easy to see that

$$y_n = y_m \prod_{k=m+1}^n a_k + Y_{n,m}$$

where $Y_{n,m}$ only depends on $b_{m+1}, b_{m+2}, \dots, b_n$ and $a_{m+2}, a_{m+3}, \dots, a_n$ and not on y_m . It is possible to give an explicit expression for $Y_{n,m}$, but we do not need this. If we assume that the relative error on the initial value y_m is bounded by the machine precision ϵ , and that computations are done in exact arithmetic (i.e. without roundoff errors), then it follows that the relative error δ_m^n on y_n , computed starting from y_m , is bounded by

$$|\delta_m^n| \leq \left| \frac{\prod_{k=1}^n a_k}{y_n} \frac{y_m}{\prod_{j=1}^m a_j} \right| \epsilon. \quad (3)$$

For the case where $m > n$, we use the recurrence in the other direction, but the error analysis leads to the same result as (3). So if we want to compute y_n for $n = 0, 1, \dots, s$, we could use forward recurrence, taking $m = 0$, or backward recurrence, taking $m = s$, or a combination of both, starting from an intermediate value $0 < m < s$. If we make a logarithmic plot of the error curves (as a function of n) for different values of m (as was done in Figure 1), then these curves should be equal to each other, apart from a vertical shift. This follows easily from equation (3). The obvious approach now is to find the value of m which actually pushes the entire error curve below the machine precision level. This occurs if we take $m = n_{\max}$, where n_{\max} is the value of n which maximises the function

$$f(n) = \left| \frac{\prod_{k=1}^n a_k}{y_n} \right|.$$

We can then use this value n_{\max} to compute a whole range of solutions up to machine precision. Of course, the success of this algorithm depends on how well we can solve this maximisation problem.

3 Application to the incomplete gamma function

For our case we take $y_n = \Gamma(-x - n, \mathbf{i}y)$. Using (2) we obtain

$$y_n = \frac{-1}{x + n} \left[y_{n-1} - (\mathbf{i}y)^{-x-n} e^{-\mathbf{i}y} \right]$$

so the function $f(n)$ from the previous section is given by

$$f(n) = |\Gamma(-x - n, \mathbf{i}y)(x + 1)_n|^{-1}$$

where $(x + 1)_n$ is equal to

$$(x + 1)_n = \prod_{k=1}^n (x + k) = \frac{\Gamma(x + 1 + n)}{\Gamma(x + 1)}.$$

Making the substitution $t = x + n$, ignoring the factor $\Gamma(x + 1)$ (which does not have an influence on the location of the maximum), and noting that maximising $f(n)$ is the same as minimising $1/f(n)$, we are left with the following problem:

Find the value of $t > 0$ which minimises the function

$$g_y(t) = |\Gamma(-t, \mathbf{i}y)| \Gamma(t + 1),$$

given the real number y .

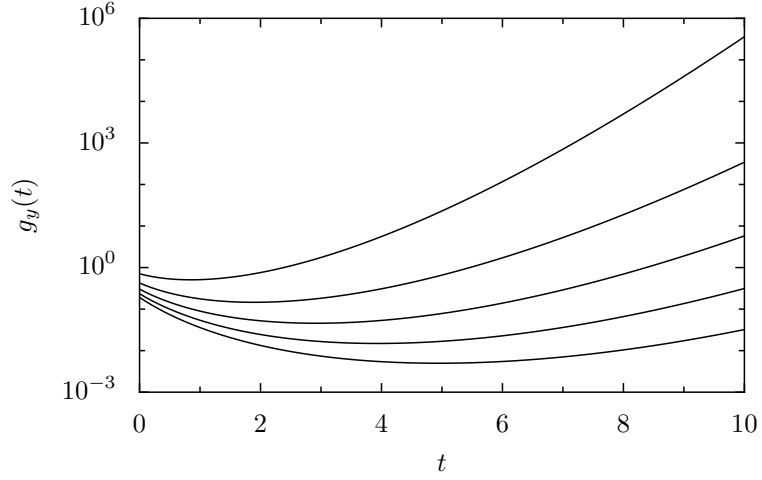


Figure 2: The function $g_y(t)$ for $y = 1, 2, \dots, 5$. The upper curve corresponds to $y = 1$, the lower one to $y = 5$.

In Figure 2 we plot $g_y(t)$ for different values of y . It seems that the minimum occurs more or less at the point $t \approx y$. This will be confirmed in the next section.

To find the (local) minima of the function $g_y(t)$, we have to solve the equation $g'_y(t) = 0$. If we write $\Gamma(-t, \mathbf{i}y) = |\Gamma(-t, \mathbf{i}y)| \exp(\mathbf{i}\theta(t, y))$ then we may reason as follows (the prime always denotes differentiation with respect to t),

$$\begin{aligned} g'_y(t) &= \Gamma'(-t, \mathbf{i}y) e^{-\mathbf{i}\theta(t, y)} \Gamma(t+1) - \mathbf{i}\theta'(t, y) g_y(t) + \Psi(t+1) g_y(t) \\ &= \Re \left\{ \frac{\Gamma'(-t, \mathbf{i}y)}{\Gamma(-t, \mathbf{i}y)} - \mathbf{i}\theta'(t, y) + \Psi(t+1) \right\} g_y(t) \\ &= \left(\Re \left\{ \frac{\Gamma'(-t, \mathbf{i}y)}{\Gamma(-t, \mathbf{i}y)} \right\} + \Psi(t+1) \right) g_y(t), \end{aligned}$$

where \Re is the real part (the second equation follows from the fact that $g'_y(t)$ is real) and $\Psi(t)$ is the digamma function, $\Psi(t) = \Gamma'(t)/\Gamma(t)$. So we are eventually lead to the equation

$$\Re \left\{ \frac{\Gamma'(-t, \mathbf{i}y)}{\Gamma(-t, \mathbf{i}y)} \right\} + \Psi(t+1) = 0. \quad (4)$$

The analytical treatment of this equation is very difficult for two reasons. First of all, the derivative of the incomplete gamma function with respect

to its *first* argument is cumbersome to deal with (quite contrary to the derivative with respect to the second argument, which is very simple). This is similar to the case of the ordinary gamma function, whose derivative is usually studied through another special function, the digamma function. Note that the argument of \Re is some kind of ‘incomplete digamma function’. Secondly, we have to take the real part, which means splitting the incomplete gamma function and its derivative in real and imaginary parts. This will introduce products of Böhmer integrals [3, p. 149] and their derivatives, which does not exactly simplify matters. Therefore we will only tackle this problem *asymptotically*, for large values of y , and then check numerically whether this approximation is good enough for *all* values of y .

4 Analysis based on uniform asymptotic expansions

It is our aim in this section to show that the solution to (4) satisfies

$$t = y + O(y^{-1}), \quad y \rightarrow \infty.$$

First note that we can limit our attention to the case $y > 0$ because it is easily proved that $g_{-y}(t) = g_y(t)$. So in what follows we assume that $y > 0$. We cannot use the well-known asymptotic expansion for $\Gamma(a, z)$ as given in [1, p. 263],

$$\Gamma(a, z) \sim z^{a-1} e^{-z} \left[1 + \frac{a-1}{z} + \dots \right], \quad z \rightarrow \infty,$$

because it is only valid if z tends to infinity for fixed a such that $|a| \ll |z|$, while in our case Figure 2 indicates that $|a| \approx |z|$. Therefore we will use the uniform asymptotic expansions from [9] to perform the analysis. This has the disadvantage, however, that the computations become much more complicated.

Uniform asymptotic expansions for the incomplete gamma function have been studied by Temme in [7, 8, 9]. In the last reference, the author studies expansions for the function $\Gamma(-t, -z)$ as t tends to infinity in $|\arg t| < \pi$. We briefly summarise his results.

For $\lambda > 0$ define η as

$$\frac{1}{2}\eta^2 = \lambda - 1 - \log \lambda, \quad \text{sign}(\eta) = \text{sign}(\lambda - 1). \quad (5)$$

This relation can be extended to complex values by analytic continuation. Next define

$$\Gamma^*(t) = \sqrt{t/(2\pi)} e^t t^{-t} \Gamma(t)$$

then it can be shown that

$$\Gamma^*(t) \sim \sum_{n=0}^{\infty} (-1)^n \frac{\gamma_n}{t^n} \quad \text{and} \quad \frac{1}{\Gamma^*(t)} \sim \sum_{n=0}^{\infty} \frac{\gamma_n}{t^n}, \quad t \rightarrow \infty, \quad |\arg t| < \pi, \quad (6)$$

where the first few γ_n are given by

$$\gamma_0 = 1, \quad \gamma_1 = -\frac{1}{12}, \quad \gamma_2 = \frac{1}{288}, \quad \gamma_3 = \frac{139}{51840}.$$

Using these γ_n we can recursively define the expansion coefficients

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

Then with $\lambda = z/t$ it follows from formula (3.6) [9] that

$$-\Gamma(t+1) \frac{e^{\pi i a}}{2\pi i} \Gamma(-t, ze^{\pi i}) = \frac{1}{2} \operatorname{erfc}\left(\mathbf{i}\eta\sqrt{\frac{t}{2}}\right) - \mathbf{i} \frac{e^{\frac{1}{2}t\eta^2}}{\sqrt{2\pi t}} T_t(\eta), \quad (7)$$

where $\operatorname{erfc}(z)$ is the complementary error function

$$\operatorname{erfc}(z) = \frac{2}{\sqrt{\pi}} \int_z^{\infty} e^{-t^2} dt$$

and the function $T_t(\eta)$ satisfies the asymptotic expansion

$$T_t(\eta) \sim \sum_{n=0}^{\infty} (-1)^n \frac{C_n(\eta)}{t^n}, \quad t \rightarrow \infty$$

uniformly with respect to $|\arg t| \leq \pi - \delta_1$ and $|\arg \lambda| \leq 2\pi - \delta_2$, with δ_1, δ_2 arbitrarily small positive constants. The first few terms are given by

$$T_t(\eta) \sim \frac{1}{\lambda - 1} - \frac{1}{\eta} - \left(\frac{1}{\eta^3} - \frac{\lambda}{(\lambda - 1)^3} + \frac{\gamma_1}{\lambda - 1} \right) \frac{1}{t} + O(t^{-2}), \quad t \rightarrow \infty \quad (8)$$

Furthermore, it can be shown that this function satisfies the differential equation

$$\frac{d}{d\eta} T_t(\eta) + t\eta T_t(\eta) = t \left(\frac{\eta}{\lambda - 1} \Gamma^*(t) - 1 \right). \quad (9)$$

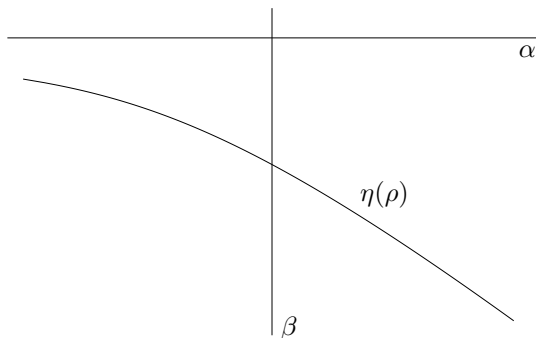


Figure 3: The function $\eta(\rho)$ in the complex plane. As ρ increases from 0 to infinity, the curve is traversed from left to right.

Now we use the previous uniform asymptotic expansion to study the behaviour of the solution to equation (4). Differentiating (7) with respect to t and using formulas (5) and (9), we obtain after some calculations that

$$\frac{d}{dt}\Gamma(-t, ze^{\pi i}) = -\Psi(t+1)\Gamma(-t, ze^{\pi i}) - \pi i\Gamma(-t, ze^{\pi i}) + \frac{2\pi e^{-\pi i t + \frac{1}{2}t\eta^2}}{\Gamma(t+1)\sqrt{2\pi t}} \left[-\frac{\eta}{2} - \frac{\eta^2}{2}T_t(\eta) + \frac{1}{2t}T_t(\eta) + \Gamma^*(t) \right].$$

Putting $z = -iy$, substituting the above expression in (4) and again using (7) we are then led to the equation

$$\Im \left\{ \frac{\eta + \eta^2 T_t(\eta) - \frac{1}{t}T_t(\eta) - 2\Gamma^*(t)}{\mathbf{i}\sqrt{\frac{2}{\pi t}}T_t(\eta) - e^{-\frac{1}{2}t\eta^2} \operatorname{erfc}\left(\mathbf{i}\eta\sqrt{\frac{t}{2}}\right)} \right\} = 0 \quad (10)$$

(note that this is still exact, since we have not yet used any asymptotic approximations). To solve this equation asymptotically, we want to use the well-known expansion for erfc as given by formula 7.1.23 in [1, p. 298]. But first we study in some more detail the relation (5) between $\lambda = -iy/t$ for $y, t > 0$, and η , to make sure that we are indeed allowed to use this expansion. If we put $\rho = y/t$ and $\eta = \alpha + \mathbf{i}\beta$, we may proceed as in section 5 of [8] and obtain the equations

$$\begin{aligned} \alpha^2 - \beta^2 &= -2(1 + \log \rho), \\ \alpha\beta &= -\rho + \pi/2. \end{aligned}$$

With the branch of the square root implied by (5), these can be solved to yield

$$\alpha = \operatorname{sign}\left(\rho - \frac{\pi}{2}\right) \sqrt{-(1 + \log \rho) + \sqrt{(1 + \log \rho)^2 + (\rho - \pi/2)^2}},$$

$$\beta = -\sqrt{1 + \log \rho + \sqrt{(1 + \log \rho)^2 + (\rho - \pi/2)^2}}.$$

Figure 3 shows the curve $\eta(\rho)$ as ρ goes from 0 to infinity. The most important thing to note is that η is bounded away from 0 for every value of ρ . This means that

$$\lim_{t \rightarrow \infty} \left| \eta \sqrt{\frac{t}{2}} \right| = \infty,$$

uniformly in y . It also follows from the above equations (and from the figure) that

$$\left| \arg \left(\mathbf{i} \eta \sqrt{\frac{t}{2}} \right) \right| < \frac{\pi}{2} < \frac{3\pi}{4}.$$

The last two formulas indicate that both conditions from [1, p. 298] for the asymptotic expansion of erfc are satisfied, so we may write

$$e^{-\frac{1}{2}t\eta^2} \operatorname{erfc} \left(\mathbf{i} \eta \sqrt{\frac{t}{2}} \right) \sim -\mathbf{i} \sqrt{\frac{2}{\pi t}} \frac{1}{\eta} \left(1 + \frac{1}{\eta^2 t} + O(t^{-2}) \right), \quad t \rightarrow \infty.$$

Combining this with the expansions (8) for $T_t(\eta)$ and (6) for $\Gamma^*(t)$ and doing some algebra, we can transform equation (10) into

$$\Re \left\{ \frac{\log \lambda - \left(\frac{1}{2} \frac{\lambda+1}{\lambda-1} + \frac{\lambda \log \lambda}{(\lambda-1)^2} - \gamma_1 \log \lambda \right) \frac{1}{t} + O(t^{-2})}{1 + \left(\frac{\lambda}{(\lambda-1)^2} - \gamma_1 \right) \frac{1}{t} + O(t^{-2})} \right\} = 0. \quad (11)$$

Remember that $\lambda = -\mathbf{i}y/t$. If we assume that the solution $t(y)$ to equation (11) satisfies an expansion of the form

$$t(y) = a_1 y + a_0 + \frac{a_{-1}}{y} + \frac{a_{-2}}{y^2} + \dots, \quad y \rightarrow \infty,$$

(where the a_i are real numbers), then it easily follows that $a_1 = 1$. Substituting $t = y + a_0 + O(y^{-1})$ in the above equation and computing a series expansion for $y \rightarrow \infty$ gives

$$\Re \left\{ -\frac{1}{2} \mathbf{i} \pi - \left(a_0 + \frac{1}{2} \mathbf{i} + \frac{5}{12} \mathbf{i} \pi \right) \frac{1}{y} + O(y^{-2}) \right\} = 0$$

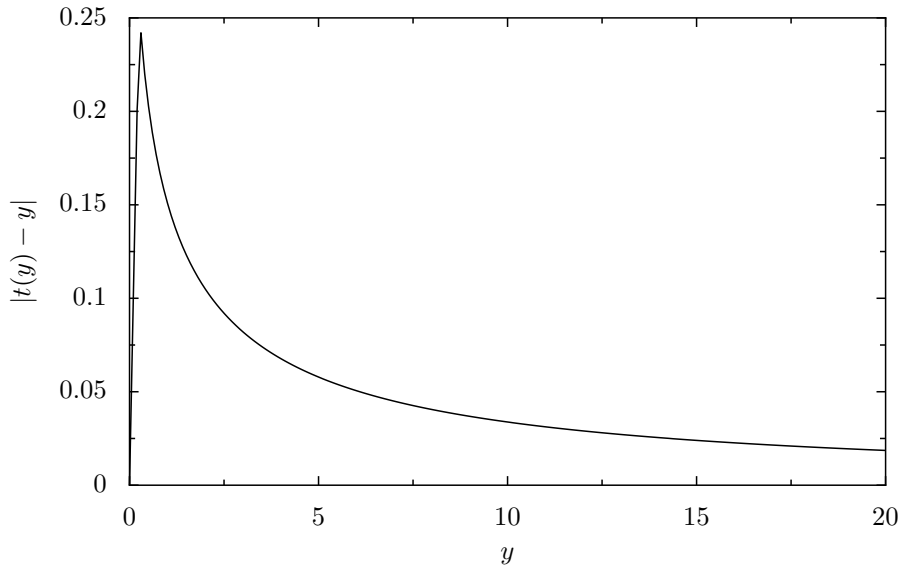


Figure 4: Distance between the exact solution $t(y)$ of the minimisation problem and the approximation $t \approx y$.

from which it follows that $a_0 = 0$ (doing these computations by hand is quite cumbersome; we used a computer algebra package to obtain the results). This effectively shows that

$$t = y + O(y^{-1}), \quad y \rightarrow \infty.$$

If we want to compute more of the a_i coefficients, we have to take more terms in the expansions for $T_t(\eta)$, $\Gamma^*(t)$ and erfc , but then the computations soon become extremely complicated because of the appearance of the η 's.

5 Accuracy of the asymptotic solution

Figure 4 shows a plot of the function $|t(y) - y|$ for $y \in (0, 20]$. The values of $t(y)$ were computed in Matlab 7 using the function `fminbnd` with the constraint $t \geq 0$, for 200 different values of y in the interval $(0, 20]$. It is clear that the approximation becomes better as $y \rightarrow \infty$. But more interesting is that the approximation error never seems to exceed 0.25. The strange behaviour on the left of the graph is due to the constraint $t \geq 0$. For a certain value y_0 , the exact solution to (4) will equal 0 and if $y < y_0$, then

x	y	bi – dir $n = \lceil y - x \rceil$	forward $n = 0$	backward $n = s$
1	1	$2.09e - 15$	$2.09e - 15$	$2.02e + 142$
1	25.5	$2.04e - 14$	$1.04e - 06$	$4.15e + 12$
1	50	$4.89e - 14$	$1.55e + 04$	$7.64e - 06$
13.25	1	$2.00e - 15$	$2.00e - 15$	$7.55e + 157$
13.25	25.5	$2.23e - 14$	$1.33e - 13$	$1.38e + 20$
13.25	50	$6.24e - 14$	$7.71e - 07$	$3.39e - 02$
25.5	1	$8.88e - 16$	$8.88e - 16$	$9.33e + 167$
25.5	25.5	$1.97e - 14$	$1.97e - 14$	$8.72e + 28$
25.5	50	$4.33e - 14$	$1.55e - 11$	$3.27e + 03$
37.75	1	$8.88e - 16$	$8.88e - 16$	$1.22e + 176$
37.75	25.5	$2.11e - 14$	$2.11e - 14$	$1.04e + 36$
37.75	50	$6.08e - 14$	$2.65e - 13$	$1.03e + 09$
50	1	$1.11e - 15$	$1.11e - 15$	$3.84e + 182$
50	25.5	$1.29e - 14$	$1.29e - 14$	$1.44e + 43$
50	50	$4.23e - 14$	$4.23e - 14$	$1.32e + 14$

Table 1: Maximum relative error using recurrence in both directions, forward and backward for $s = 100$ and different values of x and y .

$t < 0$, which we do not allow. Because of this constraint, `fminbnd` returns $t = 0$ if $y < y_0$ so the left part of the graph is just equal to $|y|$. We come back to the restriction $t \geq 0$ later.

Remember from section 3 that we are actually looking for the *integer* $n = \lceil t(y) - x \rceil$ for given x and y (where we use the symbol $\lceil \cdot \rceil$ to indicate rounding to the nearest integer). Since the approximation error for $t(y)$ does not exceed 0.25, the exact n will not differ more than 1 from the approximation $\lceil y - x \rceil$. This is perfectly acceptable.

In the rest of this section we give some numerical examples where we compute

$$\Gamma(-x - j, \mathbf{i}y), \quad j = 0, 1, \dots, s \quad (12)$$

for different values of x , y and s , using the recurrence formula. We start this recurrence from the value $\Gamma(-x - n, \mathbf{i}y)$ where $n = \lceil |y| - x \rceil$ and work in both directions. Obviously, if n is outside the range $[0, s]$, we take either $n = 0$ or $n = s$. It is assumed that the initial value is known up to machine precision, which is approximately $2.22 \cdot 10^{-16}$. In our examples it is computed using the continued fraction representation of $\Gamma(a, z)$ as explained in [11].

Table 1 shows the maximum relative error over the entire range (12)

for $s = 100$ and different values of x and y . We also show the error using forward and backward recurrence, starting from $\Gamma(-x, iy)$ and $\Gamma(-x - s, iy)$ respectively. It is clear from this table that our approach is indeed the correct approach, yielding almost all correct digits for all cases we tested.

6 Conclusion

In this paper we presented a method to compute the incomplete gamma function over a wide range of values (12) using the recurrence formula without any loss of correct digits. This method, in fact, works for any function satisfying a two term recurrence relation, provided that an accurate estimate is available (or can easily be computed) for the argument which maximises the relative error. We restricted our attention to the case $x > 0$, because for negative x the function $g_y(x)$ of section 3 has several local minima (due to the poles of $\Gamma(x + 1)$) and our simple estimate for the global minimum is no longer valid.

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