A Computational Procedure for Incomplete Gamma Functions

WALTER GAUTSCHI
Purdue University

We develop a computational procedure, based on Taylor's series and continued fractions, for evaluating Tricomi's incomplete gamma function $\gamma^*(a, x) = (x^{-a}/\Gamma(a))\int_0^x e^{-t}t^{a-1}\,dt$ and the complementary incomplete gamma function $\Gamma(a, x) = \int_x^\infty e^{-t}t^{a-1}\,dt$, suitably normalized, in the region $x \geq 0$, $-\infty < a < \infty$.

Key Words and Phrases: computation of incomplete gamma functions, Taylor's series, continued fractions
CR Categories: 5.12
The Algorithm: Incomplete Gamma Functions. *ACM Trans. Math. Software 5,* 4(Dec. 1979), 482-489.

1. INTRODUCTION

The incomplete gamma function and its complementary function are usually defined by

$$\gamma(a, x) = \int_0^x e^{-t}t^{a-1}\,dt, \qquad \Gamma(a, x) = \int_x^\infty e^{-t}t^{a-1}\,dt. \tag{1.1}$$

By Euler's integral for the gamma function,

$$\gamma(a, x) + \Gamma(a, x) = \Gamma(a). \tag{1.2}$$

We are interested in computing both functions for arbitrary x, a in the half-plane

$$\mathcal{H} = \{(x, a) : x \geq 0, -\infty < a < \infty\}.$$

The function $\Gamma(a, x)$ is meaningful everywhere in $\mathcal{H}$, except along the negative a-axis, where it becomes infinite. The definition of $\gamma(a, x)$ is less satisfactory, inasmuch as it requires $a > 0$. The difficulty, however, is easily resolved by adopting Tricomi's version [14] of the incomplete gamma function,

$$\gamma^*(a, x) = \frac{x^{-a}}{\Gamma(a)}\gamma(a, x), \tag{1.3}$$

This work was supported in part by the U.S. Army under Contract DAAG29-75-C-0024 and in part by the National Science Foundation under Grant MCS 76-00842.
Author's address. Department of Computer Sciences, Purdue University, Mathematical Sciences Building, Room 442, West Lafayette, IN 47907.

which can be continued analytically into the entire (x, a)-plane, resulting in an entire function both in a and x,

$$\gamma^*(a, x) = \frac{e^{-x}M(1, a + 1; x)}{\Gamma(a + 1)} = \frac{M(a, a + 1; -x)}{\Gamma(a + 1)}. \tag{1.4}$$

Here,

$$M(a, b; z) = 1 + \frac{a}{b}\frac{z}{1!} + \frac{a(a + 1)}{b(b + 1)}\frac{z^2}{2!} + \cdots$$

is Kummer's function. Moreover, $\gamma^*(a, x)$ is real-valued for a and x both real, in contrast to $\Gamma(a, x)$, which becomes complex for negative x.

Our objective, then, is to compute the functions $\gamma^*(a, x)$ and $\Gamma(a, x)$, suitably normalized, to any prescribed accuracy for arbitrary x, a in $\mathscr{H}$. We do not attempt here to compute $\gamma^*(a, x)$ for negative x, which may well be a more difficult (but, fortunately, less important) task. We accomplish our task by selecting one of the two functions as *primary function*, to be computed first, and computing the other in terms of the primary function by means of

$$\Gamma(a, x) = \Gamma(a)\{1 - x^a\gamma^*(a, x)\} \tag{1.5}$$

or

$$\gamma^*(a, x) = x^{-a}\left\{1 - \frac{\Gamma(a, x)}{\Gamma(a)}\right\}. \tag{1.6}$$

If $\gamma^*(a, x)$ is the primary function, we evaluate it by Taylor's series. For $\Gamma(a, x)$ we use a combination of methods, including direct evaluation based partly on power series, recursive computation, and the classical continued fraction of Legendre. Although our procedure is valid throughout the region $\mathscr{H}$, excessively large values of a and x will strain it, particularly when $a \doteq x \gg 1$ (cf. Section 5). In such cases it may be preferable to use asymptotic methods, e.g. the uniform asymptotic expansions of Temme [12]. We shall not consider these here, however, nor do we implement them in our algorithm.

An evaluation procedure of the generality attempted here is likely to be of interest in many diverse areas of application. Widely used special cases of $\gamma^*(a, x)$ or $\Gamma(a, x)$ include Pearson's form of the incomplete gamma function [10],

$$I(u, p) = (u\sqrt{p + 1})^{p+1}\gamma^*(p + 1, u\sqrt{p + 1}), \qquad u \geq 0, \quad p > -1, \tag{1.7}$$

the χ^2-probability distribution functions

$$P(\chi^2 \mid \nu) = \left(\frac{1}{2}\chi^2\right)^{\nu/2}\gamma^*\left(\frac{\nu}{2}, \frac{1}{2}\chi^2\right), \qquad Q(\chi^2 \mid \nu) = \frac{1}{\Gamma(\nu/2)}\Gamma\left(\frac{\nu}{2}, \frac{1}{2}\chi^2\right), \tag{1.8}$$

the exponential integrals

$$E_\nu(x) = x^{\nu-1}\Gamma(-\nu + 1, x) \tag{1.9}$$

(which, for $\nu = -n$, a negative integer, yield the molecular integrals $A_n(x)$ [7]), and the error functions

$$\operatorname{erf} x = x\gamma^*(\tfrac{1}{2}, x^2), \qquad \operatorname{erfc} x = (1/\sqrt{\pi})\Gamma(\tfrac{1}{2}, x^2). \tag{1.10}$$

When a is integer-valued, $\gamma^*(a, x)$ becomes an elementary function,

$$\gamma^*(-n, x) = x^n, \qquad \gamma^*(n+1, x) = x^{-(n+1)}[1 - e^{-x}e_n(x)], \quad n = 0, 1, 2, \ldots, \tag{1.11}$$

where $e_n(x) = \sum_{k=0}^{n} x^k/k!$.

2. NORMALIZATION AND ASYMPTOTIC BEHAVIOR

The purpose of normalizing functions is twofold: In the first place, one wants to scale the function in such a way that underflow or overflow on a computer is avoided in as large a region as possible. In the second place, one wants to bring the function into a form in which it is used most naturally and conveniently in applications. There is little doubt as to what the proper normalization ought to be for $\Gamma(a, x)$ and $\gamma^*(a, x)$, when a is a positive number. The formulas (1.7), (1.8), (1.10), and (1.11), indeed, all point toward the normalization

$$G(a, x) = \frac{\Gamma(a, x)}{\Gamma(a)}, \qquad g^*(a, x) = x^a\gamma^*(a, x), \quad 0 \le x < \infty, \ a > 0. \tag{2.1}$$

We then have, by (1.5),

$$G(a, x) + g^*(a, x) = 1, \quad 0 \le x < \infty, \ a > 0.$$

It is equally clear that division by $\Gamma(a)$ to normalize $\Gamma(a, x)$, when a is negative or zero, is undesirable, as this would generate functions identically zero for $x > 0$, when a is integer-valued, and would cause complications in evaluating exponential and molecular integrals (cf. (1.9)). Growth considerations, on the other hand, suggest a multiplicative factor $e^x x^{-a}$. The function $\gamma^*(a, x)$ behaves rather capriciously for $a < 0$ and is not easily normalized. We decided (somewhat reluctantly) to adopt the same normalization as in (2.1), primarily for reasons of uniformity and good behavior for large a and x. We are doing this, however, at the expense of introducing a singularity along the line $x = 0$. For nonpositive a, we thus define

$$G(a, x) = e^x x^{-a}\Gamma(a, x), \qquad g^*(a, x) = x^a\gamma^*(a, x), \quad 0 \le x < \infty, \ a \le 0. \tag{2.2}$$

Our efforts will be directed towards computing $G(a, x)$ and $g^*(a, x)$ in the region $\mathscr{H}$.

It is useful to briefly indicate the behavior of $G(a, x)$ and $g^*(a, x)$ in the various parts of the region $\mathscr{H}$. The limit values, as x approaches zero for fixed a, are readily found to be

$$\begin{aligned} &G(a, 0) = 1, && g^*(a, 0) = 0 \quad \text{if } a > 0, \\ &G(a, 0) = \infty, && g^*(a, 0) = 1 \quad \text{if } a = 0, \\ &G(a, 0) = 1/|a|, && g^*(a, 0) = \infty \quad \text{if } a < 0. \end{aligned} \tag{2.3}$$

(It should be noted that $g^*(a, x)$, considered as a function of two independent variables, is indeterminate at $a = 0$, $x = 0$.) If $|a|$ is bounded and x large, we

deduce from well-known asymptotic formulas [13, p. 174],

$$\begin{aligned} G(a, x) &\sim \frac{e^{-x}x^{a-1}}{\Gamma(a)}, \quad a > 0 \text{ bounded}, \\ G(a, x) &\sim \frac{1}{x}, \qquad a \leq 0 \text{ bounded}, \quad x \to \infty. \\ g^*(a, x) &\sim 1, \qquad |a| \text{ bounded}, \end{aligned} \tag{2.4}$$

Equally simple is the case $|x|$ bounded and $a \to \infty$ (over positive values of a), in which case [13, p. 175]

$$\begin{aligned} G(a, x) &\sim 1, \qquad |x| \text{ bounded}, \\ & \qquad\qquad\qquad a(>0) \to \infty. \\ g^*(a, x) &\sim \frac{e^{-x}x^a}{\Gamma(a+1)}, \quad |x| \text{ bounded}, \end{aligned} \tag{2.5}$$

An indication of the behavior of these functions, when both variables are large, can be gained by setting $x = \rho a$, $\rho > 0$ fixed, and letting $a \to \infty$. Laplace's method, applied to the integrals in (1.1), then gives

$$G(a, \rho a) \sim \begin{cases} 1, & 0 < \rho < 1, \\ \frac{1}{2}, & \rho = 1, \qquad a \to \infty, \\ \dfrac{\rho^a e^{-(\rho-1)a}}{\sqrt{2\pi a}\,(\rho - 1)}, & \rho > 1, \end{cases}$$

$$g^*(a, \rho a) \sim \begin{cases} \dfrac{\rho^a e^{(1-\rho)a}}{\sqrt{2\pi a}\,(1 - \rho)}, & 0 < \rho < 1, \\ \frac{1}{2}, & \rho = 1, \qquad a \to \infty. \\ 1, & \rho > 1, \end{cases} \tag{2.6}$$

Similarly,

$$G(-a, \rho a) \sim \frac{1}{(\rho + 1)a}, \quad 0 < \rho < \infty, \; a \to \infty,$$

$$g^*(-a, \rho a) \sim \begin{cases} \dfrac{2 \sin \pi a}{\sqrt{2\pi a}\,(\rho + 1)} \rho^{-a} e^{-a(\rho+1)} & \text{if } \rho e^{\rho+1} < 1, \\ a \not\equiv 0 \pmod 1, \qquad a \to \infty. \\ 1 \quad \text{if } \rho e^{\rho+1} \geq 1, \end{cases} \tag{2.7}$$

3. CHOICE OF PRIMARY FUNCTION

Either of the two functions $\Gamma(a, x)$, $\gamma^*(a, x)$ can be expressed in terms of the other by means of the relations

$$\Gamma(a, x) = \Gamma(a)\{1 - x^a\gamma^*(a, x)\}, \qquad \gamma^*(a, x) = x^{-a}\left\{1 - \frac{\Gamma(a, x)}{\Gamma(a)}\right\}. \tag{3.1}$$

In our choice of primary function, we are guided primarily by considerations of numerical stability. We must be careful not to lose excessively in accuracy when

we perform the subtractions indicated in braces in (3.1). No such loss occurs if the absolute value of the respective difference is larger than, or equal to, $\frac{1}{2}$. This criterion is easily expressed in terms of the ratio

$$r(a, x) = \frac{\Gamma(a, x)}{\Gamma(a)}. \tag{3.2}$$

Indeed, the first relation in (3.1) is stable exactly if $|r(a, x)| \geq \frac{1}{2}$, while the second is stable in either of the two cases $r(a, x) \geq \frac{3}{2}$ and $r(a, x) \leq \frac{1}{2}$. As a consequence, *an ideal choice of the primary function is* $\gamma^*(a, x)$ *if* $\frac{1}{2} \leq r(a, x) \leq \frac{3}{2}$, *and* $\Gamma(a, x)$ *if* $|r(a, x)| \leq \frac{1}{2}$; *in all remaining cases either choice is satisfactory.*

For the practical implementation of this criterion, consider first $a > 0$, $x > 0$. In this case, $0 < r(a, x) < 1$, and $r(a, x)$ increases monotonically in the variable a ([14, p. 276]). Since $\lim_{a\to 0} r(a, x) = 0$ and, by (2.5), $\lim_{a\to\infty} r(a, x) = 1$, there is a unique curve $a = \alpha(x)$ in the first quadrant $x > 0$, $a > 0$, along which $r(a, x) = \frac{1}{2}$, and $r(a, x) \gtrless \frac{1}{2}$ depending on whether $a \gtrless \alpha(x)$. Since, by (2.6), $r(x, x) \sim \frac{1}{2}$ as $x \to \infty$, we have $\alpha(x) \doteq x$ for x large. By numerical computation it is found that in fact $\alpha(x) \doteq x$ for all (except very small) positive x, the value of $\alpha(x)$ consistently being slightly larger than x. As $x \to 0$ one finds $\alpha(x) \sim \ln \frac{1}{2}/\ln x$, which suggests the approximation $\alpha(x) \doteq \alpha^*(x)$, where

$$\alpha^*(x) = \begin{cases} x + \frac{1}{4}, & \frac{1}{4} \leq x < \infty, \\ \ln \frac{1}{2}/\ln x, & 0 < x \leq \frac{1}{4}. \end{cases} \tag{3.3}$$

The proper choice of primary function thus is $\Gamma(a, x)$ (resp. $G(a, x)$) if $0 < a \leq \alpha(x)$, and $\gamma^*(a, x)$ (resp. $g^*(a, x)$) if $a > \alpha(x)$, where $\alpha(x)$ may be approximated by $\alpha^*(x)$ in (3.3).

In the case $a \leq 0$, $x > 0$, the second relation in (3.1) is stable if $\Gamma(a) < 0$, i.e. if

$$-m - 1 < a < -m, \tag{3.4}$$

where $m \geq 0$ is an even integer. If $m \geq 1$ is an odd integer and a as in (3.4), then for x not too large there is a possibility that $\gamma^*(a, x)$ will vanish. The second relation in (3.1) is then subject to cancellation errors. A similar problem of cancellation, however, would occur if $\gamma^*(a, x)$ were calculated directly (e.g. from its Taylor expansion in the variable x). Furthermore, if $\gamma^*(a, x)$ were the primary function, the first relation in (3.1) would create serious (though not unsurmountable) computational difficulties for values of a near (or equal!) to a nonpositive integer (cf. the relevant discussion in [3]). All these considerations lead us to adopt $\Gamma(a, x)$ (resp. $G(a, x)$) as the primary function, whenever $a \leq 0$.

In summary, then, *our choice of primary function is* $\Gamma(a, x)$ *(resp.* $G(a, x)$*), if* $-\infty < a \leq \alpha(x)$, *and* $\gamma^*(a, x)$ *(resp.* $g^*(a, x)$*), if* $a > \alpha(x)$. Here, $\alpha(x)$ is adequately approximated by $\alpha^*(x)$ in (3.3).

4. THE COMPUTATION OF $G(a, x)$

As discussed in Section 3, it suffices to consider the region $-\infty < a \leq \alpha^*(x)$, $x \geq 0$. We shall break up this region into the following three subregions:

Region I: $0 \leq x \leq x_0$, $-\frac{1}{2} \leq a \leq \alpha^*(x)$.
Region II: $0 \leq x \leq x_0$, $-\infty < a < -\frac{1}{2}$.
Region III: $x > x_0$, $-\infty < a \leq \alpha^*(x)$.

The breakpoint x_0 will be chosen to have the value $x_0 = 1.5$. (A motivation for this choice is given in subsection 4.1.) We use a different method of computation in each of these three subregions. In Region I we first compute $\Gamma(a, x)$ directly from (1.4) and (1.5), and then use (2.1) or (2.2), depending on whether $a > 0$ or $a \leq 0$, to obtain $G(a, x)$. In Region II we employ a recurrence relation in the variable a, the starting value being computed by the method appropriate for Region I (except, possibly, when $x < \frac{1}{4}$). In Region III we use a continued fraction due to Legendre. We now proceed to describe and justify these various methods in more detail.

4.1 Direct Computation of $\Gamma(a, x)$ and $G(a, x)$ for $0 < x \leq x_0$, $-\frac{1}{2} \leq a \leq a^*(x)$

Using (1.5), we can write

$$\Gamma(a, x) = \Gamma(a) - \frac{x^a}{a} + \frac{x^a}{a}[1 - \Gamma(a + 1)\gamma^*(a, x)]. \tag{4.1}$$

We let

$$u = \Gamma(a) - \frac{x^a}{a},$$
$$v = \frac{x^a}{a}[1 - \Gamma(a + 1)\gamma^*(a, x)], \tag{4.2}$$

and propose to use

$$\Gamma(a, x) = u + v \tag{4.3}$$

as a basis of computation in Region I. The breakpoint x_0 will be determined, among other things, from the requirement that the relative error generated in (4.3) (due to respective errors in u and v) be within acceptable limits.

Before analyzing these errors, we observe that both quantities u and v have finite limits as $a \to 0$, when $x > 0$. Indeed,

$$\lim_{a \to 0} u = -\gamma - \ln x, \qquad \lim_{a \to 0} v = E_1(x) + \gamma + \ln x, \tag{4.4}$$

where $\gamma = .57721...$ is Euler's constant and $E_1(x)$ is the exponential integral. The first relation follows at once from

$$u = \frac{\Gamma(1 + a) - 1}{a} - \frac{x^a - 1}{a}, \tag{4.5}$$

the second from (4.3) by letting $a \to 0$ and noting that $\Gamma(0, x) = E_1(x)$. Furthermore, from (1.1) and (1.3), we have

$$v = \int_0^x t^{a-1}(1 - e^{-t})dt, \tag{4.6}$$

valid not only for $a > 0$, but even for $a > -1$. In particular, therefore,

$$v > 0 \quad \text{if } a > -1, x > 0. \tag{4.7}$$

Using Taylor's expansion in (4.6) it is possible to compute v very accurately, essentially to machine precision. The same can be said for u, except that near the

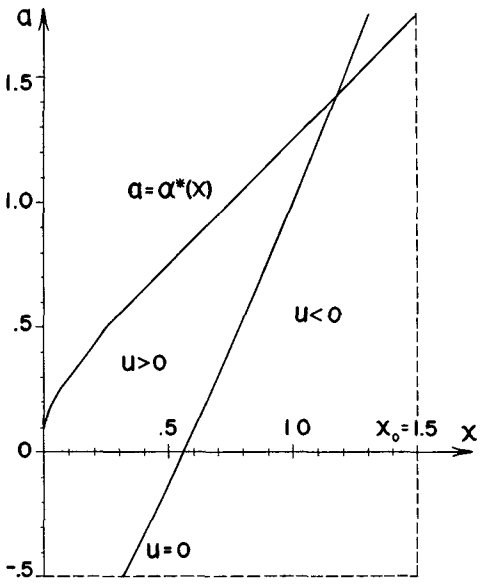

Fig. 1. The subregions $u \gtrless 0$ in Region I

line where $u = 0$ (see Figure 1) the precision will be attained only in terms of the absolute error, not the relative error. If the absolute and relative error of u is e_u and ϵ_u, respectively, and ϵ_v is the relative error of v, then the relative error ϵ_Γ of $\Gamma(a, x)$, computed by (4.3), will be

$$\epsilon_\Gamma = \frac{e_u + v\epsilon_v}{u + v} = \frac{u\epsilon_u + v\epsilon_v}{u + v}.$$

Therefore, if $\epsilon = \max(|\epsilon_u|, |\epsilon_v|)$, we have, in view of (4.7),

$$|\epsilon_\Gamma| \leq \epsilon \quad \text{if} \quad u > 0, \qquad |\epsilon_\Gamma| \leq \left(1 + \frac{2|u|}{u + v}\right)\epsilon \quad \text{if} \quad u < 0. \tag{4.8}$$

Similarly, if $e = \max(|e_u|, |\epsilon_v|)$, then

$$|\epsilon_\Gamma| \leq \frac{1 + v}{u + v}\, e. \tag{4.9}$$

It is seen from the first relation in (4.8) that (4.3) is perfectly stable if $u > 0$, except possibly when u is very close to zero, in which case the absolute (not relative) error of u is what matters. Even then, however, one finds that the error magnification in (4.3) is negligible, since along the line $u = 0$ in Region I the factor $1 + 1/v$ multiplying e in (4.9) is always less than 3.8. In the subregion $u < 0$ of Region I it has been determined by computation[1] that the magnification factor

$$\mu(a, x) = 1 + \frac{2|u|}{u + v}$$

[1] A preliminary version of an algorithm for computing $\Gamma(a, x)$ and $\gamma^*(a, x)$ (see [3]) was used for this purpose.

Table I Maximum Error Magnification in Formula (4.3)

x_0	0.5	1.0	1.5	2.0	2.5	3.0
$\mu(-\frac{1}{2}, x_0)$	3.426	18.34	56.25	142.6	327.3	706.5

in (4.8) decreases monotonically as a function of a. It is easily verified, moreover, that in the same subregion the quantity $\mu(a, x)$ increases monotonically as a function of x. Therefore, the maximum error magnification occurs at the corner $(-\frac{1}{2}, x_0)$ of Region I. Table I shows the value of μ at this corner point in dependence on x_0. A similar behavior is exhibited by the magnification factor in (4.9). Its values at $(-\frac{1}{2}, x_0)$, however, are generally smaller than those in Table I.

Since the continued fraction used in Region III converges rather more slowly when x gets small, we have an interest in choosing x_0 as large as possible. Unfortunately, this runs counter the increased instability of (4.3). By way of a compromise, we will adopt the value $x_0 = 1.5$, thus accepting a possible loss of between 1 and 2 decimal digits. This choice of x_0 also strikes a reasonable balance in the computational work on either side of the boundary line separating Region III from Region I.

For the actual computation of u, we use (4.5) when $|a| < \frac{1}{2}$ and the first of (4.2), otherwise. The term in (4.5) involving the gamma function will be written in the form

$$\frac{\Gamma(1+a)-1}{a} = -\frac{1}{a}\cdot\Gamma(1+a)\cdot\left\{\frac{1}{\Gamma(1+a)}-1\right\}, \quad |a|<\frac{1}{2},$$

and evaluated using the Taylor expansions of $[\Gamma(1+a)]^{-1}$ and $[\Gamma(1+a)]^{-1}-1$, respectively. High-precision values of the necessary coefficients are available in [16, table 5]. Similarly, for the remaining term we write

$$\frac{x^a-1}{a} = \frac{e^{a\ln x}-1}{a\ln x}\cdot\ln x,$$

and evaluate the first factor on the right by Taylor expansion whenever $|a \ln x| < 1$.

The computation of v is most easily accomplished by series expansion. From (4.6) we find immediately

$$v = -x^a \sum_{n=1}^{\infty} \frac{(-x)^n}{(a+n)n!}, \quad a > -1, \tag{4.10}$$

or, equivalently,

$$v = \frac{x^{a+1}}{a+1}\sum_{k=0}^{\infty} t_k, \qquad t_k = \frac{(a+1)(-x)^k}{(a+k+1)(k+1)!}, \quad k = 0, 1, 2, \ldots.$$

The terms t_k can be obtained recursively by

$$t_0 = 1, \qquad t_k = -\frac{(a+k)x}{(a+k+1)(k+1)}\,t_{k-1}, \quad k = 1, 2, 3, \ldots.$$

In an effort to reduce the number of arithmetic operations, we define $p_k = (a + k)x$, $q_k = (a + k + 1)(k + 1)$, $r_k = a + 2k + 3$, and generate $\{t_k\}$ by means of

$$p_0 = ax, \quad q_0 = a + 1, \quad r_0 = a + 3, \quad t_0 = 1,$$

$$\left.\begin{aligned} p_k &= p_{k-1} + x, \\ q_k &= q_{k-1} + r_{k-1}, \\ r_k &= r_{k-1} + 2, \\ t_k &= -p_k \cdot t_{k-1}/q_k, \end{aligned}\right\} \quad k = 1, 2, 3, \ldots.$$

This requires only three additions, one multiplication, and one division per iteration step.

It is worth noting that overflow poses no serious threat in computing $\Gamma(a, x)$ as described. Indeed, $\Gamma(a, x)$ decreases in x, hence is largest along the left boundary of Region I. The respective boundary values are finite, equal to $\frac{1}{2}\Gamma(a) = (1/2a)\Gamma(a + 1)$, if $a > 0$, and infinite, if $a \leq 0$. As $x \to 0$ for fixed $a \leq 0$, $\Gamma(a, x)$ behaves like $E_1(x) \sim -\gamma - \ln x$, if $a = 0$, and like $-x^a/a$, if $a < 0$. In all cases ($a > 0$, and $-\frac{1}{2} < a \leq 0$) the values of $\Gamma(a, x)$ are machine representable if a, $1/a$, and x are.

Having computed $\Gamma(a, x)$, one obtains $G(a, x)$ from the first relations in (2.1) and (2.2), according as $a > 0$ or $a \leq 0$, respectively. The secondary function $g^*(a, x)$ then follows from $G(a, x)$ by

$$g^*(a, x) = \begin{cases} 1 - \dfrac{e^{-x}x^a G(a, x)}{\Gamma(a)}, & a < 0, \\ 1, \quad a = 0, & \\ 1 - G(a, x), & a > 0. \end{cases} \tag{4.11}$$

4.2 Recursive Computation of G(a, x) for $0 < x \leq x_0$, $-\infty < a < -\frac{1}{2}$

We let[2] $m = [\frac{1}{2} - a]$, so that

$$a = -m + \epsilon, \qquad -\tfrac{1}{2} < \epsilon \leq \tfrac{1}{2},$$

$$G(a, x) = G(-m + \epsilon, x),$$

where m is an integer greater than or equal to 1. Defining $G_n = G(-n + \epsilon, x)$, $n = 0, 1, 2, \ldots$, the well-known recurrence relation in the variable a, satisfied by $\Gamma(a, x)$, yields[3]

$$\begin{aligned} G_0 &= G(\epsilon, x), \\ G_n &= \frac{1}{n - \epsilon}(1 - x\,G_{n-1}), \quad n = 1, 2, \ldots, m. \end{aligned} \tag{4.12}$$

[2] The symbol $[r]$ denotes the largest integer less than or equal to r.

[3] The normalization (2.2) for $G(\epsilon, X)$ must be adopted here, even if $\epsilon > 0$.

The error propagation pattern in (4.12) is very similar for all ϵ in $-\frac{1}{2} < \epsilon \leq \frac{1}{2}$. When x is small ($x \lesssim 0.2$), the error is consistently damped for all n. When x is larger, there is an initial interval $1 \leq n \leq n_0$ in which the error is amplified, and a subsequent interval $n > n_0$ of rapid error damping. As x increases, both n_0 and the maximum error amplification increases. The latter, however, is well within acceptable limits, if $x \leq x_0 = 1.5$, the error never being amplified by more than a factor of 5.7. The case $\epsilon = 0$, which is typical, is analyzed in [5, example 5.4 and fig. 3]. (Note, in this connection, that $G(-m, x) = e^x E_{m+1}(x)$, where $E_{m+1}(x)$ is the exponential integral of order $m + 1$.) The recurrence relation (4.12), therefore, is extremely stable in the region in which it is being used.

The initial value $G_0 = G(\epsilon, x)$ can be computed by the method appropriate for Region I (see Section 4.1), except when $x < \frac{1}{4}$ and $\epsilon > \alpha^*(x)$, in which case $g^*(\epsilon, x)$ is computed first (see Section 5), whereupon $G(\epsilon, x)$ is obtained in a stable manner from $g^*(\epsilon, x)$, using $G(\epsilon, x) = \Gamma(\epsilon)e^x x^{-\epsilon}(1 - g^*(\epsilon, x))$ (cf. footnote 3).

4.3 Computation of G(a, x) for $x > x_0$, $-\infty < a \leq \alpha^*(x)$ by Legendre's Continued Fraction

The following continued fraction, due to Legendre, is well known ([11, p. 103; 1, eq. 6.5.31]),

$$x^{-a}e^x\Gamma(a, x) = \frac{1}{x+}\ \frac{1-a}{1+}\ \frac{1}{x+}\ \frac{2-a}{1+}\ \frac{2}{x+}\cdots. \tag{4.13}$$

It converges for any $x > 0$ and for arbitrary real a. We can write (4.13) in contracted form as

$$x^{-a}e^x\Gamma(a, x) = \frac{\beta_0}{x + \alpha_0 +}\ \frac{\beta_1}{x + \alpha_1 +}\ \frac{\beta_2}{x + \alpha_2 +}\cdots,$$

$$\alpha_k = 2k + 1 - a, \qquad k = 0, 1, 2, \ldots,$$

$$\beta_0 = 1, \qquad \beta_k = k(a - k), \qquad k = 1, 2, 3, \ldots,$$

or, alternatively, in the form

$$(x + 1 - a)x^{-a}e^x\Gamma(a, x) = \frac{1}{1+}\ \frac{a_1}{1+}\ \frac{a_2}{1+}\ \frac{a_3}{1+}\cdots, \tag{4.14}$$

where

$$a_k = \frac{k(a - k)}{(x + 2k - 1 - a)(x + 2k + 1 - a)}, \qquad k = 1, 2, 3, \ldots. \tag{4.15}$$

We investigate the convergence character of the continued fraction in (4.14) for $x > x_0 = 1.5$, $-\infty < a \leq \alpha^*(x)$, which is Region III, in which (4.14) is going to be used.

It is well known (cf., e.g. [15, p. 17ff]) that any continued fraction of the form (4.14) can be evaluated as an infinite series,

$$\frac{1}{1+}\,\frac{a_1}{1+}\,\frac{a_2}{1+}\,\frac{a_3}{1+}\cdots = \sum_{k=0}^{\infty} t_k, \tag{4.16}$$

where

$$t_0 = 1, \qquad t_k = \rho_1\rho_2\cdots\rho_k, \qquad k = 1, 2, 3, \ldots, \tag{4.17}$$

$$\rho_0 = 0, \qquad \rho_k = \frac{-a_k(1+\rho_{k-1})}{1+a_k(1+\rho_{k-1})}, \qquad k = 1, 2, 3, \ldots. \tag{4.18}$$

The nth partial sum in (4.16), in fact, is equal to the nth convergent of the continued fraction, $n = 1, 2, 3, \ldots$. If we let $\sigma_k = 1 + \rho_k$, then the recursion for ρ_k in (4.18) translates into the following recursion for σ_k:

$$\sigma_0 = 1, \quad \sigma_k = \frac{1}{1 + a_k\sigma_{k-1}}, \quad k = 1, 2, 3, \ldots. \tag{4.19}$$

Consider now the case of a_k as given in (4.15). If $k < a$ (thus $a > 1$), then $a_k > 0$ (since $a \le x + \frac{1}{4}$), and it follows inductively from (4.19) that $0 < \sigma_k < 1$; hence $-1 < \rho_k < 0$. In view of (4.17), this means that (4.16) initially behaves like an alternating series with terms decreasing monotonically in absolute value.

If $k > a$, then $a_k < 0$, and σ_k may become larger than 1. However, if $0 < \sigma_{k-1} \le 2$, we claim that $1 < \sigma_k \le 2$ whenever $x \ge \frac{1}{4}$. Indeed, for the upper bound we must show that $1 + a_k\sigma_{k-1} \ge \frac{1}{2}$, i.e. $a_k\sigma_{k-1} \ge -\frac{1}{2}$, or, equivalently, $|a_k|\sigma_{k-1} \le \frac{1}{2}$. Since $\sigma_{k-1} \le 2$, it suffices to show $|a_k| \le \frac{1}{4}$, which is equivalent to $1 \le (x-a)^2 + 4kx$. Since $k \ge 1$ and $x > 0$, the latter is certainly true if $x \ge \frac{1}{4}$, which proves the assertion $\sigma_k \le 2$. The other inequality, $1 < \sigma_k$, is an easy consequence of $1 + a_k\sigma_{k-1} > 0$, established in the course of the argument just given, and the negativity of a_k. Since for the first k with $k > a$ we have $0 < \sigma_{k-1} \le 1$ (by virtue of the discussion in the preceding paragraph, or by virtue of $\sigma_0 = 1$), it follows inductively that $1 < \sigma_k \le 2$ for all $k > a$, hence $0 < \rho_k \le 1$. In the case $k = a$, we have $a_k = 0$ and $\sigma_k = 1$, thus $\rho_k = 0$, and the argument again applies.

We have shown that $|\rho_k| \le 1$ for all $k \ge 1$, that is, the terms in the series of (4.16) are nonincreasing in modulus, whenever $-\infty < a \le \alpha^*(x)$, $x \ge \frac{1}{4}$, in particular, therefore, when (x, a) is in Region III under consideration. Moreover, the series changes from an alternating series (if $a > 1$), initially, to a monotone series, ultimately.

In the region $a > \alpha^*(x)$, convergence of Legendre's continued fraction may deteriorate considerably in speed, which, together with the appropriate choice of primary function, is the reason we prefer a different method for $a > \alpha^*(x)$ (cf. Section 5).

Computationally, the summation in (4.16), with the a_k given in (4.15), can be simplified similarly as in (4.10). We now define $p_k = -k(a-k)$, $q_k = (x + 2k - 1 - a)(x + 2k + 1 - a)$, $r_k = 4(x + 2k + 1 - a)$, $s_k = 2k - a + 1$, and generate the terms t_k in (4.16) by means of

$$p_0 = 0, \quad q_0 = (x - 1 - a)(x + 1 - a), \quad r_0 = 4(x + 1 - a),$$
$$s_0 = -a + 1, \quad \rho_0 = 0, \quad t_0 = 1,$$

$$\left.\begin{aligned} p_k &= p_{k-1} + s_{k-1} \\ q_k &= q_{k-1} + r_{k-1} \\ r_k &= r_{k-1} + 8 \\ s_k &= s_{k-1} + 2 \\ \tau_k &= p_k(1 + \rho_{k-1}) \\ \rho_k &= \frac{\tau_k}{q_k - \tau_k} \\ t_k &= \rho_k t_{k-1} \end{aligned}\right\} \quad k = 1, 2, 3, \ldots. \tag{4.20}$$

This requires six additions, two multiplications, and one division per term.

5. THE COMPUTATION OF $g^*(a, x) = x^a\gamma^*(a, x)$

We need to consider only the region $a > \alpha^*(x)$, $x \geq 0$, in which $g^*(a, x)$ is the primary function (cf. Section 3). Among the tools available for computing $\gamma^*(a, x)$ are the two power series

$$\Gamma(a + 1)e^x\gamma^*(a, x) = e^x \sum_{n=0}^{\infty} \frac{a(-x)^n}{(a + n)n!} = \Gamma(a + 1) \sum_{n=0}^{\infty} \frac{x^n}{\Gamma(a + n + 1)}, \tag{5.1}$$

which follow immediately from (1.4), and the continued fraction

$$\Gamma(a + 1)e^x\gamma^*(a, x) = \frac{1}{1-} \quad \frac{x}{a + 1 + x -} \quad \frac{(a + 1)x}{a + 2 + x -} \quad \frac{(a + 2)x}{a + 3 + x -} \cdots, \tag{5.2}$$

which can be derived from Perron's continued fraction for ratios of Kummer functions [4]. In our preliminary work [3] we used the first series in (5.1), if $x \leq 1.5$, and the continued fraction (5.2), if $x > 1.5$. Our preference for the alternating series in (5.1) was motivated by the fact that $\gamma^*(a, x)$ in [3] served as primary function in the whole strip $0 \leq x \leq 1.5$, $-\infty < a < \infty$. In this case the first series in (5.1) has the advantage of terminating after the first term, if $a = 0$, and of presenting similar simplifications if a is a negative integer. These advantages had to be reconciled with problems of internal cancellation, which increase as x gets larger. In the present setup, these considerations become irrelevant, and indeed for $a > \alpha^*(x)$ the second series in (5.1) is clearly more attractive, all terms being positive (hence no cancellation), and convergence being quite rapid, even for x relatively large (in which case $a > x + \frac{1}{2}$).

How does this series compare with the continued fraction (5.2)? Rather surprisingly, the answer is: They are identical! In other words, the successive convergents of the continued fraction are identical with the successive partial sums of the series. To see this, let A_n, B_n be the numerators and denominators of the continued fraction in (5.2), so that, in particular,

$$B_1 = 1, \qquad B_2 = a + 1,$$

$$B_n = (a + n - 1 + x)B_{n-1} - (a + n - 2)xB_{n-2}, \quad n = 3, 4, \ldots.$$

One easily verifies by induction that

$$B_1 = 1, \qquad B_n = (a + 1)(a + 2) \cdots (a + n - 1), \quad n = 2, 3, \ldots. \tag{5.3}$$

From the theory of continued fractions it is known that

$$\frac{A_n}{B_n} - \frac{A_{n-1}}{B_{n-1}} = (-1)^{n-1} \frac{a_1 a_2 \cdots a_n}{B_{n-1}B_n},$$

where $a_1 = 1$, $a_2 = -x$, $a_n = -(a + n - 2)x$ $(n > 2)$ are the partial numerators in (5.2). It follows, by virtue of (5.3), that

$$\frac{A_n}{B_n} - \frac{A_{n-1}}{B_{n-1}} = \frac{x^{n-1}}{(a + 1)(a + 2) \cdots (a + n - 1)}, \quad n \geq 2;$$

hence

$$\frac{A_n}{B_n} = 1 + \sum_{k=2}^{n} \left(\frac{A_k}{B_k} - \frac{A_{k-1}}{B_{k-1}} \right) = 1 + \sum_{k=2}^{n} \frac{x^{k-1}}{(a + 1)(a + 2) \cdots (a + k - 1)},$$

which is the nth partial sum of the series on the far right of (5.1).

Since series are easier to compute than continued fractions, we propose to compute $g^*(a, x)$ by

$$g^*(a, x) = x^a e^{-x} \sum_{n=0}^{\infty} \frac{x^n}{\Gamma(a + n + 1)} \tag{5.4}$$

everywhere in the region $a > \alpha^*(x)$.

The use of (5.4) in the region $a > \alpha^*(x)$ is comparable, with regard to computational effort, to the use of Legendre's continued fraction in the neighboring region $a < \alpha^*(x)$, $x > 1.5$, except when x is very large and $a \doteq \alpha^*(x)$, in which case Legendre's continued fraction is more efficient. Some pertinent data are shown in Table II. We determined the number of iterations required for 8 decimal digit accuracy in Legendre's continued fraction (4.14), when $a = \alpha^*(x)(1 - h)$, and in the power series (5.4), when $a = \alpha^*(x)(1 + h)$, where h was given the values 0.001, 0.25, 0.5, 0.75, 1.0, 1.5, 2.0, 2.5, 3.0, and $x = 10, 20, 40, 80, \ldots, 10240$. Table II shows for each x the minimum and maximum number of iterations

Table II. Number of Iterations in Legendre's Continued Fraction (4.14) and in Taylor's Expansion (5.4) for 8-Digit Accuracy

	$x = 10$		$x = 20$		$x = 40$		$x = 80$		$x = 160$		$x = 320$	
	min	max	min	max	min	max	min	max	min	max	min	max
Legendre	7	10	6	15	5	19	4	25	4	32	3	41
Taylor	13	24	13	31	14	42	14	57	14	77	14	106
	$x = 640$		$x = 1280$		$x = 2560$		$x = 5120$		$x = 10240$			
Legendre	3	52	3	65	3	82	2	101	2	124		
Taylor	14	146	14	202	14	279	14	387	14	536		

as h varies over the values specified. The number of iterations consistently decreases with increasing $|h|$, so that the maximum occurs on the boundary line $a = \alpha^*(x)$. In order to properly evaluate the data in Table II, one must keep in mind that each iteration in Legendre's continued fraction, using the algorithm in (4.20), requires seven additions, two multiplications, and one division, whereas each iteration in Taylor's series requires only two additions, one multiplication, and one division. Thus, Legendre's continued fraction is $2 - 2\frac{1}{2}$ times as expensive, per iteration, as Taylor's series.

6. TESTING

The algorithm in [2] and a double precision version of it were tested extensively on the CDC 6500 computer at Purdue University against a double precision version of the procedure in [3]. The double precision algorithms were used to provide reference values for checking the single precision algorithm, and on a few occasions, to check against high precision tables (notably the 14S tables in [8]). Other reference values were taken from various mathematical tables in the literature.

The tests include:

(i) the error functions (1.10), checked against tables 7.1 and 7.3 in [1];
(ii) the case (1.11) of integer values $a = n$, $-20 \leq n \leq 20$;
(iii) the exponential integral $E_\nu(x)$ in (1.9) for integer values $\nu = n$, $0 \leq n \leq 20$, and fractional values of ν in $0 \leq \nu \leq 1$, checked against tables I, II, III in [9];
(iv) Pearson's incomplete gamma function (1.7), checked against tables I and II in [10];
(v) the incomplete gamma function $P(a, x) = (x/2)^a\gamma^*(a, x/2)$, checked against the tables in [6];
(vi) the χ^2 distribution (1.8), checked against table 26.7 in [1];
(vii) the molecular integral $A_n(x)$, checked against table 1 in [7] and the more accurate tables in [8].

An important feature of our algorithm is the automatic monitoring of overflow and underflow conditions. This is accomplished by first computing the logarithm of the desired quantities and by making the tests for overflow and underflow on the logarithms. As a result, minor inaccuracies are introduced in the final exponentiation, which become particularly noticeable if the result is near the overflow or underflow limit.

7. SEQUENCES OF INCOMPLETE GAMMA FUNCTIONS

Expansions in terms of incomplete gamma functions require the generation of sequences $G_n = G(\alpha + n, x)$ or $g_n^* = g^*(\alpha + n, x)$ for fixed α and $n = 0, 1, 2, \ldots$, or of suitably scaled sequences $\{\lambda_n G_n\}$, $\{\lambda_n^* g_n^*\}$, where $\lambda_n \neq 0$, $\lambda_n^* \neq 0$ are scale factors. (For the purpose of the following discussion, the choice of these factors is immaterial; we shall assume, therefore, $\lambda_n = \lambda_n^* = 1$.) It would be wasteful to compute the G_n and g_n^* individually, for each n, by some evaluation procedure (such as the one developed in Sections 3–5). More efficient is the use of recurrence

relations satisfied by G_n and g_n^*. We discuss this in the case $\alpha > 0$, $x > 0$, which is a case of practical importance.

7.1 Generation of $G_n = G(\alpha + n, x)$

From the difference equation $G(a + 1, x) = G(a, x) + x^a e^{-x}/\Gamma(a + 1)$, letting $a = \alpha + n$, one finds immediately the recurrence relation

$$G_{n+1} = G_n + \frac{x^{\alpha+n}e^{-x}}{\Gamma(\alpha + n + 1)}, \quad n = 0, 1, 2, \ldots. \tag{7.1}$$

The numerical stability of (7.1) is determined by the solution $h_n = 1$ of the associated homogeneous recurrence relation, through the "amplification factors" [5]

$$\rho_n = \left|\frac{G_0 h_n}{G_n}\right| = \frac{\Gamma(\alpha, x)}{\Gamma(\alpha)}\frac{\Gamma(\alpha + n)}{\Gamma(\alpha + n, x)}. \tag{7.2}$$

Indeed, if s and t are arbitrary nonnegative integers, a small (relative) error ϵ injected into (7.1) at $n = s$ will propagate into a (relative) error $\epsilon\rho_t/\rho_s$ at $n = t$, causing the error to be damped if $\rho_t < \rho_s$ and magnified if $\rho_t > \rho_s$. To achieve consistent error damping, hence perfect numerical stability, the recurrence relation (7.1) ought to be applied *in the direction of decreasing* ρ_n.

Since $\Gamma(a, x)/\Gamma(a)$ increases from 0 to 1 on the interval $0 < a < \infty$ [14, p. 276], we see from (7.2) that ρ_n decreases monotonically from 1 to $\Gamma(\alpha, x)/\Gamma(\alpha)$, as n increases from 0 to ∞. It follows that *the recurrence relation* (7.1) *is perfectly stable in the forward direction.* The proper way to compute the sequence $\{G_n\}$, therefore, consists in first evaluating $G_0 = G(\alpha, x)$ (using our evaluation procedure, for example), and then applying (7.1) for $n = 0, 1, 2, \ldots$ to successively generate as many of the G_n as desired.

7.2 Generation of $g_n^* = g_n^*(\alpha + n, x)$

From the difference equation $g^*(a + 1, x) = g^*(a, x) - x^a e^{-x}/\Gamma(a + 1)$, we now find the recurrence relation

$$g_{n+1}^* = g_n^* - \frac{x^{\alpha+n}e^{-x}}{\Gamma(\alpha + n + 1)}, \quad n = 0, 1, 2, \ldots, \tag{7.3}$$

which has associated the amplification factors

$$\rho_n^* = \left|\frac{g_0^* h_n^*}{g_n^*}\right| = \frac{\gamma(\alpha, x)}{\Gamma(\alpha)}\frac{\Gamma(\alpha + n)}{\gamma(\alpha + n, x)}, \tag{7.4}$$

since $h_n^* = 1$ and $g_n^* = \gamma(\alpha + n, x)/\Gamma(\alpha + n)$. Noting that $\Gamma(a, x)/\Gamma(a) = 1 - \gamma(a, x)/\Gamma(a)$, and that the ratio on the left increases monotonically from 0 to 1 as a function of a, it follows that $\gamma(a, x)/\Gamma(a)$ decreases monotonically from 1 to 0, hence that ρ_n^* increases monotonically from 1 to ∞ as n increases from 0 to ∞. Therefore, *the recurrence relation* (7.3) *is perfectly stable in the backward direction.* Wishing to compute g_n^* for $n = 0, 1, 2, \ldots, N$, say, we should therefore use our evaluation procedure on $g_N^* = g^*(\alpha + N, x)$, and then employ (7.3) in the

form

$$g_n^* = g_{n+1}^* + \frac{x^{\alpha+n}e^{-x}}{\Gamma(\alpha + n + 1)}, \quad n = N - 1, N - 2, \ldots, 0,$$

to generate all remaining values of g_n^*.

ACKNOWLEDGMENT

The author is indebted to N. M. Temme for suggesting the approach in Sections 4.1 and 4.2.

REFERENCES

1. ABRAMOWITZ, M., AND STEGUN, I.A., EDS. *Handbook of Mathematical Functions.* Nat. Bur. Standards Appl. Math. Series 55, U.S. Govt. Printing Office, 1964.
2. GAUTSCHI, W. Algorithm 542. Incomplete gamma functions. *ACM Trans. Math. Software 5,* 4 (Dec. 1979), 482–489.
3. GAUTSCHI, W. An evaluation procedure for incomplete gamma functions. MRC Tech. Summary Rep. 1717, Mathematics Res. Ctr., U. of Wisconsin, Madison, Feb. 1977.
4. GAUTSCHI, W Anomalous convergence of a continued fraction for ratios of Kummer functions. *Math. Comp. 31* (1977), 994–999.
5. GAUTSCHI, W Zur Numerik rekurrenter Relationen. *Comptg. 9* (1972), 107–126. (English translation in Aerospace Res. Lab. Rep. ARL 73-0005, Wright Patterson AFB, Feb. 1973.)
6. KHAMIS, S H. *Tables of the Incomplete Gamma Function Ratio.* Justus von Liebig Verlag, Darmstadt, 1965.
7. KOTANI, M., AMENIYA, A., ISHIGURO, E., AND KIMURA, T. *Table of Molecular Integrals.* Maruzen Co , Ltd., Tokyo, 1955
8. MILLER, J., GERHAUSEN, J.M., AND MATSEN, F.A. *Quantum Chemistry Integrals and Tables* U. of Texas Press, Austin, 1959.
9. PAGUROVA, V I. *Tables of the Exponential Integral* $E_p(x) = \int_1^\infty e^{-xu}u^{-p}\,du$. (Translated from the Russian by D. G. Fry), Pergamon Press, New York, 1961.
10. PEARSON, K., Ed., *Tables of the Incomplete* Γ*-Function* Biometrika Office, U. College, Cambridge U. Press, Cambridge, 1934.
11. PERRON, O. *Die Lehre von den Kettenbruchen, Vol. II,* 3rd ed., B.G. Teubner, Stuttgart, 1957.
12. TEMME, N.M. The asymptotic expansion of the incomplete gamma functions. Rep. TW 165/77, Stichting Mathematisch Centrum, Amsterdam, 1977.
13. TRICOMI, F.G. Funzioni ipergeometriche confluenti. Edizioni Cremonese, Rome, 1954.
14 TRICOMI, F.G. Sulla funzione gamma incompleta. *Ann. Mat. Pura Appl. (4) 31* (1950), 263–279.
15. WALL, H.S. *Analytic Theory of Continued Fractions* Van Nostrand, New York, 1948. (Reprinted in 1967 by Chelsea Publ Co., Bronx, N.Y)
16. WRENCH, J.W., JR. Concerning two series for the gamma function. *Math. Comp. 22* (1968), 617–626.

Received April 1977, revised August 1978