# ON THE COMPUTATION OF THE INCOMPLETE GAMMA FUNCTIONS FOR LARGE VALUES OF THE PARAMETERS

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A method for computing incomplete gamma functions is given for the case when the parameters are both positive and large. The method is based on earlier results of the author on uniform asymptotic expansions of these functions. It is concluded that the method may be considered as an addition to Gautschi's algorithm, which becomes inefficient in the case that the method described here is best applicable.

## 1. INTRODUCTION

For the computation of special functions of mathematical physics or mathematical statistics, polynomial or rational min-max approximations are frequently used. These methods are especially efficient when a single real argument has to be considered. In multivariate problems, or when complex variables are involved, analytical expansions and representations are preferred. Key words are: recurrence relations, continued fraction, series expansions. See, for instance, [ 2 ] , [ 4 ] and [ 5 ] for details on this topic.

In this paper we consider the use of an asymptotic representation for incomplete gamma functions, functions of two variables which are assumed to be non-negative. Essential in our approach is the fact that we do not use the asymptotic expansion of the functions involved. Instead we use a series expansion, the coefficients of which are generated by a simple recursion. In this way it is possible to construct an algorithm for the incomplete gamma function for the difficult case, i.e. when both parameters are large. Comparing our method with existing algorithms we observe a remarkable reduction in computational effort.

## 2. DEFINITIONS AND NOTATIONS

We use the incomplete gamma functions in the normalized form

$$P(a,x) = \frac{1}{\Gamma(a)} \int_0^x t^{a-1} e^{-t} dt, \quad Q(a,x) = \frac{1}{\Gamma(a)} \int_x^\infty t^{a-1} e^{-t} dt \tag{2.1}$$

with $x \geq 0$ and $a > 0$. By this definition,

$$P(a,x) + Q(a,x) = 1. \tag{2.2}$$

So, in the computational problem we compute the one of (2.1) that is less than $\frac{1}{2}$, and (2.2) gives the other one. With slight corrections for small values of x and a we have the following rule:

$0 \leq a \leq x$: first compute Q, then $P = 1-Q$;

$0 \leq x < a$: first compute P, then $Q = 1-P$.

This follows from the asymptotic relation

$$P(a,a),\ Q(a,a) \sim \frac{1}{2},\ a\to\infty.$$

A rather complete discussion of the computational problem for P and Q is given in [3]. The method for Q is based on Legendre's continued fraction (x not too small) and the method for P on the Taylor series

$$P(a,x) = x^a e^{-x} \sum_{n=0}^{\infty} \frac{x^n}{\Gamma(a+n+1)}. \tag{2.3}$$

Gautschi reports, for 8-digit accuracy with x = 10240 and $a = x.(1+0.001)$, the need in the power series of 536 terms, and for $a = x.(1-0.001)$ of 124 iterations for the continued fraction (with the remark that the continued fraction is 2 - $2\frac{1}{2}$ times as expensive, per iteration, as the Taylor series). Comparing this with our approach is not fair, since our method is especially suitable for large values of a and x, with $a \sim x$. Our claim is that the method presented here is a useful addition to Gautschi's procedure for a large area of the a,x- quarter plane around the diagonal $a = x$. More information on the computational effort of our method will be given in section 4.

## 3. UNIFORM ASYMPTOTIC EXPANSIONS

In [6] we obtained the following representation for P and Q

$$\begin{cases} P(a,x) = \frac{1}{2}\,\mathrm{erfc}(-\eta\sqrt{a/2}) - R_a(\eta), \\ Q(a,x) = \frac{1}{2}\,\mathrm{erfc}(\eta\sqrt{a/2}) + R_a(\eta); \end{cases} \tag{3.1}$$

erfc is the error function defined by

$$\mathrm{erfc}(z) = 2/\sqrt{\pi}\int_z^\infty e^{-t^2}\,dt. \tag{3.2}$$

The real parameter $\eta$ in (3.1) is defined by

$$\tfrac{1}{2}\eta^2 = \lambda - 1 - \ln\lambda,\ \lambda = x/a,\ \mathrm{sign}\,(\eta) = \mathrm{sign}(\lambda-1). \tag{3.3}$$

For the function $R_a(\eta)$ we derived an asymptotic expansion. Writing

$$R_a(\eta) = \frac{e^{-\frac{1}{2}a\eta^2}}{\sqrt{2\pi a}}\,S_a(\eta), \tag{3.4}$$

we have

$$S_a(\eta) \sim \sum_{n=0}^{\infty} \frac{C_n(\eta)}{a^n},\ a \to \infty, \tag{3.5}$$

$\eta \in \mathbb{R}$. No restrictions on $\eta$ are needed: it may be fixed as large as we please and it may grow with a as fast as we please. In fact, (3.5) holds uniformly with respect to $\eta \in \mathbb{R}$ (and in a larger domain of the complex plane). The first coefficients in (3.5) are

$$\begin{cases} C_0(\eta) = \frac{1}{\lambda-1} - \frac{1}{\eta}, \\ C_1(\eta) = \frac{1}{\eta^3} - \frac{1}{(\lambda-1)^3} - \frac{1}{(\lambda-1)^2} - \frac{1}{12(\lambda-1)}. \end{cases} \tag{3.6}$$

These two, and all higher coefficients, have a removable singularity at $\eta = 0$ ($\lambda = 1$, $x = a$). Consequently, the numerical evaluation is difficult for small values of $|\eta|$. Recall our remark that the area $a \sim x$ (both large) gives problems in the existing software and that our approach will concentrate on this domain.

To evaluate the coefficients $C_k(\eta)$ of (3.5) near $\eta = 0$ we can expand each coefficient in a Taylor series

$$C_k(\eta) = \sum_{n=0}^{\infty} C_n^{(k)} \eta^n, \quad k = 0, 1, \dots . \tag{3.7}$$

The series converges for $|\eta| < 2\sqrt{\pi}$. Recurrence relations for $C_n^{(k)}$ are given in [ 6 ]. However, with the expansions (3.7) we still need the summation of the asymptotic expansion (3.5). Although we derived error bounds for the remainders of this expansion we describe now a method in which $S_a(\eta)$ of (3.4) is expanded in a Taylor series instead of in an asymptotic series as in (3.5). The new approach seems to be more attractive for numerical calculations than that based on (3.5).

## 4. EVALUATION OF $S_a(\eta)$

Differentiating one of (3.1) with respect to $\eta$ gives

$$\frac{1}{a}\frac{d}{d\eta} S_a(\eta) = \eta\, S_a(\eta) - \frac{1}{\Gamma^*(a)} f(\eta) + 1 \tag{4.1}$$

with

$$f(\eta) = \frac{1}{\lambda}\frac{d\lambda}{d\eta} = \frac{\eta}{\lambda - 1}, \tag{4.2}$$

$$\Gamma^*(a) = \sqrt{a/2\pi}\, e^a a^{-a} \Gamma(a). \tag{4.3}$$

The functions $f(\eta)$ and $S_a(\eta)$ are analytic in a large domain of the complex $\eta$ - plane. Singularities nearest to the origin are $\eta_{\pm} = 2\sqrt{\pi}\exp(\pm 3\pi i/4)$. So we can expand

$$\begin{cases} S_a(\eta) = \dfrac{1}{\Gamma^*(a)} \displaystyle\sum_{m=0}^{\infty} b_m(a)\eta^m, \\ f(\eta) = 1 + \displaystyle\sum_{m=1}^{\infty} f_m \eta^m; \end{cases} \tag{4.4}$$

both expansions converge for $|\eta| < 2\sqrt{\pi}$. Substituting the expansions in (4.1) and comparing equal powers of $\eta$ we obtain

$$\begin{cases} b_1(a) = a[\Gamma^*(a)-1], \\ (m+1)b_{m+1}(a) = a[b_{m-1}(a) - f_m], \quad m \geq 1. \end{cases} \tag{4.5}$$

Moreover we have

$$b_0(a) = \Gamma^*(a)S_a(0) = \sqrt{2\pi a}\,\Gamma^*(a)[\tfrac{1}{2} - P(a,a)]. \tag{4.6}$$

Recursion (4.5) can be viewed as a first order inhomogeneous recursion relation for $\{b_{2m}(a)\}$, $\{b_{2m+1}(a)\}$ of which the first values $b_0$, $b_1$ are defined. However, the recursion in the forward direction is unstable, especially when a is large. More details to verify this will be given in the following section. For computing $\{b_m\}$ for $a \geq a_0$, where $a_0$ need not be large ($a_0 = 10$ is a suitable choice), we can use (4.5) in backward direction, with two approximate starting values $b_{2N}(a)$, $b_{2N+1}(a)$, where N is sufficiently large. From the next section it follows that a convenient start is

$$b_{2N+j}(a) = f_{2N+j+1}, \quad j = 0,1. \tag{4.7}$$

The starting value N depends on a and the required accuracy.

By using the backward recursion on (4.5) we can avoid the somewhat difficult computation of $b_0(a)$, $b_1(a)$. When we have computed $b_1(a)$, we also have $\Gamma^*(a)$ appearing in the first line of (4.5).

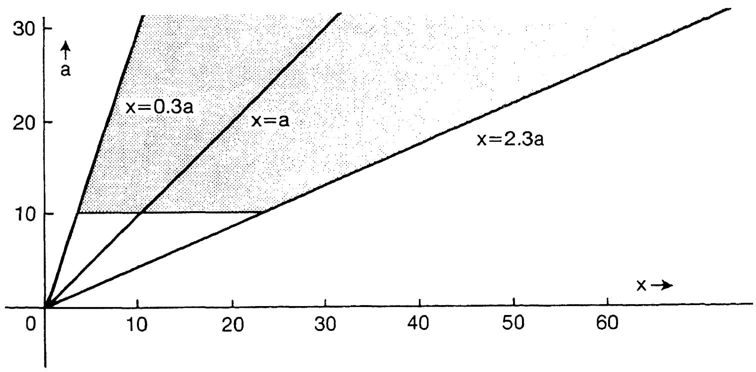


Fig. 4.1 The shaded area in the (x,a)-plane corresponds with $a \geq 10$, $\eta \in [-1,1]$.

To give an idea about the computational effort we consider the case $a = 10$ and $\eta \in [-1,1]$. We can use (4.7) with $N = 7$, and we can replace in the first line of (4.4) $\infty$ by 14 to obtain $S_a(\eta)$ within (relative) accuracy of $0.5 \times 10^{-8}$, $\eta \in [-1,1]$. So we need the pretabulation of $f_1, \ldots f_{16}$. In fact the same accuracy of 8 decimal digits is possible for all $a \in [10,\infty)$, with the same value of N, and $\eta \in [-1,1]$. For the computation of P and Q we need also the computation of the error function in (3.1). So, comparison with Gautschi's method cannot be done straightforwardly, but it will be clear now that the difficult part in (3.1), i.e., $R_a(\eta)$, can be evaluated with much less computational effort than is required in Gautschi's approach for the difficult area near $a = x$ (and both large).

Corresponding $\lambda$-values of $\eta = \pm 1$ are (see (3.3))

$$\eta = -1 : \lambda = 0.3017\ldots; \quad \eta = +1 : \lambda = 2.357\ldots. \tag{4.8}$$

It follows that $\eta \in [-1,1]$ corresponds with $x/a \in [0,3017\ldots, 2.357\ldots]$. Hence, the shaded area of the $(x,a)$-quarter plane of Figure 4.1 is covered when $a \gtrsim 10$ and $\eta \in [-1,1]$. We repeat our earlier remark that for $x,a$ in this area a pretabulation of $f_1,\ldots,f_{16}$ of (4.4) is needed and that backward recursion of (4.5) with (4.7) as starting values $(N = 7)$ gives $S_a(\eta)$ of (4.4) within 8 significant decimal digits.

From a numerical point of view more efficient approaches are possible by replacing (4.4) by Chebyshev expansions with rational functions of $\eta$ as argument of the polynomials. Much larger $\eta$-intervals can be covered then. However, the analogue of (4.5) will become more complicated.

The first few coefficients $f_m$ of (4.4) are
$f_1 = -1/3$, $f_2 = 1/12$, $f_3 = -2/135$, $f_4 = 1/864$, $f_5 = 1/2835$.
Further coefficients can be generated by the recursion

$$f_k = -\frac{k+1}{k+2}\left[\frac{(k-1)}{3k} f_{k-1} + \sum_{j=3}^{k-1} f_{j-1} f_{k+1-j}/(k+2-j)\right], \quad k \geq 4. \tag{4.9}$$

To show this we first consider the coefficients $\{\alpha_k\}$ in $\lambda = 1 + \alpha_1\eta + \alpha_2\eta^2 + \ldots$. Substituting this expansion into $(\lambda-1)d\lambda/d\eta = \lambda\eta$ (which follows from (4.2)), we obtain

$$\alpha_1 = 1,\ \alpha_2 = \frac{1}{3},\ \alpha_3 = 1/36,\ \alpha_4 = -1/270,\ \alpha_5 = 1/4320,$$

and for $k \geq 2$ the recursion

$$(k+1)\alpha_k = \alpha_{k-1} - \sum_{j=2}^{k-1} j\alpha_j\alpha_{k-j+1}. \qquad (4.10)$$

Next we observe that from (4.2) it follows that

$$f(\eta) = d(\ln\lambda)/d\eta = d(\lambda - 1 - \tfrac{1}{2}\eta^2)/d\eta = d\lambda/d\eta - \eta, \qquad (4.11)$$

which gives

$$f_1 = 2\alpha_2 - 1 = -\frac{1}{3}\ ,\ f_k = (k+1)\alpha_{k+1}\ \ (k \geq 2).$$

Using this in (4.10) we obtain (4.9).

## 5. ON THE STABILITY OF THE RECURSION FOR $\{b_m(a)\}$

To discuss the stability aspects of (4.5) we first remark that the general solution is composed of a particular solution (due to the inhomogeneous term $f_m$) and a solution of the homogeneous equation. The latter is due to the homogeneous part of (4.1), and it is the set of Taylor coefficients of $\exp(\frac{1}{2}a\eta^2)$. This exponentially large function cannot be incorporated in the solution needed here. For instance, (3.5) shows that $S_a(\eta) = O(1)$, $a \to \infty$, $\eta \in \mathbb{R}$. For the same reason the required solution of (4.5) is free of the homogeneous component $(a/2)^m/m!$, although this is very small when $m \to \infty$ (a fixed).

The Taylor series in (4.4) have equal radius of convergence. So we expect that $b_m(a)$ is of the same order as $f_m$ (when m is large) and that large values of a do not disturb this. The following analysis confirms the relation between $f_m$ and $b_m(a)$.

First we claim that $b_o(a)$ and $b_1(a)$ have the following asymptotic expansions

$$\begin{cases} b_0(a) \sim \sum_{m=0}^{\infty} 2^m m!\, f_{2m+1} a^{-m} \\ b_1(a) \sim \sum_{m=0}^{\infty} 2^m \dfrac{\Gamma(m+3/2)}{\Gamma(3/2)} f_{2m+2} a^{-m} \end{cases} \tag{5.1}$$

as $a \to \infty$, where $f_m$ are the coefficients of $f$ in (4.4).

To prove this we need more details on how (3.1) follows from (2.1). Writing $t = a\tau$ in the first of (2.1) we obtain

$$P(a,x) = \frac{1}{\Gamma^*(a)} \sqrt{\frac{a}{2\pi}} \int_0^{\lambda} e^{-a(\tau-1-\ln\tau)} \frac{d\tau}{\tau}$$

where $\Gamma^*(a)$ is given in (4.3) and $\lambda = x/a$. A further transformation $\frac{1}{2}\zeta^2 = \tau-1-\ln\tau$ (with sign $(\zeta)$ = sign $(\tau-1)$) gives

$$P(a,x) = \frac{1}{\Gamma^*(a)} \sqrt{\frac{a}{2\pi}} \int_{-\infty}^{\eta} e^{-\frac{1}{2}a\zeta^2} f(\zeta)\,d\zeta, \tag{5.2}$$

where $\eta$ is given in (3.3) and $f$ in (4.2). So, $b_0(a)$ of (4.6) can be written as

$$b_0(a) = \frac{1}{2}\sqrt{2\pi a}\,\Gamma^*(a) - a\int_{-\infty}^{0} e^{-\frac{1}{2}a\zeta^2} f(\zeta)\,d\zeta.$$

By using (5.2) with $x = \infty (\eta=\infty)$, we can write this as

$$b_0(a) = \frac{1}{2}a\int_0^{\infty} [\,f(\zeta)-f(-\zeta)\,]\,e^{-\frac{1}{2}a\zeta^2}\,d\zeta. \tag{5.3}$$

For $b_1(a)$ of (4.5) we first consider

$$\Gamma^*(a) = \sqrt{\frac{a}{2\pi}} \int_0^{\infty} [\,f(\zeta) + f(-\zeta)\,]\,e^{-\frac{1}{2}a\zeta^2}\,d\zeta. \tag{5.4}$$

By expanding $f$ as in (4.4) and substituting this in (5.3), (5.4) we obtain (5.1). By applying (4.5) we infer

$$\begin{cases} b_{2n}(a) \sim \dfrac{a^n}{2^n n!} \sum_{m=n}^{\infty} 2^m m! f_{2m+1} a^{-m} \\ b_{2n+1}(a) \sim \dfrac{a^n}{2^n \Gamma(n+3)/2)} \sum_{m=n}^{\infty} 2^m \Gamma(m+3/2) f_{2m+2} a^{-m} \end{cases} \tag{5.5}$$

as $a\to\infty$, where $n = 0,1,\ldots$ This shows that

$$b_n(a) = f_{n+1}[1 + O(a^{-1})], \quad a\to\infty, \tag{5.6}$$

which shows once again that the solution of the homogeneous part of the recursion (4.5) cannot be present in $b_n(a)$. Furthermore it makes clear why (4.7) is used for initiating the backward recursion.

The above conclusions can be based on a more rigorous analysis by introducing remainders in the expansions in (5.1). That is, we write

$$b_0(a) = \sum_{m=0}^{n-1} 2^m m! f_{2m+1} a^{-m} + 2^n n! a^{-n} r_n^{(o)}(a),$$

$$b_1(a) = \sum_{m=0}^{n-1} \frac{2^m \Gamma(m+3/2)}{\Gamma(3/2)} f_{2m+2} a^{-m} + \frac{2^n \Gamma(n+3/2)}{\Gamma(3/2)} a^{-n} r_n^{(1)}(a),$$

where $n = 0,1,\ldots,\ a > 0$. By using this representation it follows from (4.5) that

$$b_{2n}(a) = r_n^{(o)}(a), \quad b_{2n+1}(a) = r_n^{(1)}(a),$$

which is the exact interpretation of (5.5). So, the coefficients $b_n(a)$ in (4.4) are in fact the remainders of asymptotic representations of $b_0$ and $b_1$. With (4.5) the remainders are generated.

Knowing the nature of the solution of the recursion (4.5) we can now use a more explicit method to show that forward recursion is not stable. Gautschi [1] used the quantity

$$\rho_n = \frac{f_0 h_n}{f_n}, \quad n = 0,1,\ldots \tag{5.7}$$

to study the stability of the recursion

$$f_{n+1} = a_n f_n + c_n,$$

see also [4]. In (5.7) $h_n$ is the solution of the homogeneous equation $h_{n+1} = a_n h_n$, i.e.,

$$h_n = c \prod_{j=0}^{n-1} a_j,$$

where c is some constant. In our case the recursion for $\{b_{2m}\}$ gives

$$\rho_n = \frac{a^n}{2^n n!} \frac{b_0}{b_{2n}} .$$

From (5.5) and the convergence of the series in (4.4) it follows that for a first approximation we can replace $b_{2n}$ by $(2\sqrt{\pi})^{-2n}$. So we obtain

$$\rho_n = O[(\frac{2\pi ea}{n})^n], \quad n \to \infty.$$

So, given a (say a = 10), the first $\rho_n$ values are increasing very fast. There is a turning point at $n = 2\pi ea$ (=170 when a=10). This shows that backward recurrence is stable unless a is small or we need a lot of coefficients $b_m(a)$.

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