

Computing the incomplete Gamma function to arbitrary precision

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Abstract. I consider an arbitrary-precision computation of the incomplete Gamma function from the Legendre continued fraction. Using the method of generating functions, I compute the convergence rate of the continued fraction and find a direct estimate of the necessary number of terms. This allows to compare the performance of the continued fraction and of the power series methods. As an application, I show that the incomplete Gamma function $\Gamma(a, z)$ can be computed to P digits in at most $O(P)$ long multiplications uniformly in z for $\operatorname{Re} z > 0$. The error function of the real argument, $\operatorname{erf} x$, requires at most $O(P^{2/3})$ long multiplications.

1 Introduction

The incomplete Gamma function (see e.g. [1] Sec. 6.5)

$$\Gamma(a, z) = \int_z^{+\infty} t^{a-1} e^{-t} dt \quad (1)$$

is a generalization of such special functions as the Gamma function $\Gamma(a)$, the exponential integral $\operatorname{Ei} x$, and the complementary error function $\operatorname{erfc} z$. After an appropriate analytic continuation and branch cuts one obtains a definition of $\Gamma(a, z)$ valid for arbitrary complex a, z .

I consider the general problem of computing $\Gamma(a, z)$ to a precision of P (decimal) digits. Several methods have been described in the literature for the computation of the incomplete Gamma function [2–5]. However, these methods were not analyzed in view of a computation at an asymptotically high precision. In particular, the convergence rate of the Legendre continued fraction has only been checked heuristically or numerically for a particular target precision.

The purpose of this paper is to present a calculation of the convergence rate of the continued fraction of Legendre and to perform a comparative analysis of efficiency of the existing methods for an asymptotically large target precision P .

2 Overview of methods

2.1 Mathematical properties

The incomplete Gamma function admits two series expansions,

$$\Gamma(a, z) = \Gamma(a) - \sum_{n=0}^{\infty} \frac{\Gamma(a) e^{-z} z^{n+a}}{\Gamma(a+n+1)} = \Gamma(a) - \sum_{n=0}^{\infty} \frac{(-1)^n z^{n+a}}{(a+n)n!}, \quad (2)$$

an asymptotic series for large $|z|$,

$$\Gamma(a, z) = z^{a-1} e^{-z} \sum_{n=0}^{\infty} \frac{\Gamma(a)}{\Gamma(a-n)} z^{-n}, \quad (3)$$

a continued fraction expansion due to Legendre,

$$\Gamma(a, z) = \frac{e^{-z} z^a}{z+} \frac{1-a}{1+} \frac{1}{z+} \frac{2-a}{1+} \frac{2}{z+} \dots, \quad (4)$$

and a recurrence relation,

$$\Gamma(a+n+1, z) = \Gamma(a+n, z) + \frac{\Gamma(a) e^{-z} z^{n+a}}{\Gamma(a+n+1)}, \quad n \geq 0. \quad (5)$$

Both series of Eq. (2) converge unless a is a negative integer. The recurrence relation was analyzed in [4] and found to be of limited use for general a and z because of round-off errors, but usable if a is close to a negative integer. Another asymptotic expansion due to Temme [6] is cumbersome and requires costly computations of the Bernoulli numbers. Therefore we shall focus on the series expansions of Eqs. (2)-(3) and on the continued fraction. (The asymptotic series will be efficient when $|z| \gg P$.)

The error function is related to the incomplete Gamma function by $\sqrt{\pi} \operatorname{erfc} z = \Gamma(1/2, z^2)$ and has similar representations, in particular, the continued fraction due to Laplace,

$$\sqrt{\pi} x e^{x^2} \operatorname{erfc} x = \frac{1}{1+} \frac{v}{1+} \frac{2v}{1+} \frac{3v}{1+} \dots, \quad (6)$$

where $v \equiv (2x^2)^{-1}$. This representation was used e.g. in [7]. Our analysis of the continued fraction method will include Eq. (6) as a particular case.

2.2 Computation of power series

A power series $\sum_{k=1}^n b_k x^k$, where all b_k are rational numbers and x is a floating-point number with P digits, may be computed using $O(\sqrt{n})$ long multiplications using the “rectangular” or “baby step/giant step” method (see e.g. [8]). Power series of this form are most often encountered in approximations of analytic functions. The increased asymptotic speed of the “rectangular” method is obtained

when the ratios b_k/b_{k-1} are rational numbers with “short” numerators and denominators with $O(\ln k)$ digits. If these ratios are not short, the best method is the Horner scheme requiring $O(n)$ long multiplications.

The series of Eqs. (2), (3) have rational coefficients only when a is a short rational number, e.g. $a = 1/2$ for the error function. If both a and z are short rational numbers, then the series may be computed using the binary splitting method [9]. This method requires $O(\ln n)$ multiplications of $O(n \ln n)$ -digit integers and is asymptotically the fastest, albeit with limited applicability.

2.3 Computation of continued fractions

There are two main classes of methods for the numerical evaluation of continued fractions: the forward or the backward recurrences (see e.g. [10] for details of various methods). The backward recurrences are more straightforward but one needs to know the necessary number of terms n at the outset. The forward recurrences are significantly slower than the backward recurrences, but do not require to set the number of terms in advance. In our case, the number of terms can be estimated analytically and therefore the backward recurrences are preferable. The backward recurrences also have much better round-off error behavior [11]. The asymptotic complexity of all methods is $O(n)$ long multiplications.

Denote by $F_{m,n}$ the partial fraction

$$F_{m,n} = a_m + \frac{b_m}{a_{m+1} + \frac{b_{m+1}}{a_{m+2} + \dots + \frac{b_{n-1}}{a_n}}}. \quad (7)$$

There are two possible backward recurrences for $F_{m,n}$. First, one may compute the partial fractions directly,

$$F_{m,n} = a_m + \frac{b_m}{F_{m+1,n}}, \quad (8)$$

starting from $F_{n,n} = a_n$. This uses n long divisions. Second, one may compute the numerators $p_{m,n}$ and the denominators $q_{m,n}$ as separate sequences,

$$p_{m,n} = a_m p_{m+1,n} + b_m q_{m+1,n}, \quad q_{m,n} = p_{m+1,n}, \quad \left(\frac{p_{m,n}}{q_{m,n}} \equiv F_{m,n} \right) \quad (9)$$

with $p_{n,n} = a_n$, $q_{n,n} = 1$, and perform the final division $F_{0,n} = p_{0,n}/q_{0,n}$. This requires $2n$ long multiplications. Since a division usually takes at least four times longer than a multiplication [12], the latter method is faster at high precision.

A refinement of the backward recurrence method [13] is to use an ansatz for $F_{n,n}$ that more closely approximates the infinite remainder $F_{n,\infty}$ of the continued fraction. The ansatz follows from the assumption that $F_{n,\infty}$ changes slowly with n at large n ; then one finds $F_{n,\infty}$ from the equation

$$F_{n,\infty} = a_n + \frac{b_n}{F_{n,\infty}}. \quad (10)$$

Sometimes it is better to use instead the equation

$$F_{n,\infty} = a_n + \frac{b_n}{a_{n+1} + \frac{b_{n+1}}{F_{n,\infty}}}. \quad (11)$$

The validity of the ansatz for $F_{n,\infty}$ needs to be checked in each particular case. Using an ansatz for $F_{n,\infty}$ does not give an asymptotic improvement of speed, but the precision of the approximation is typically improved by several orders. One could also obtain $F_{n,\infty}$ more rigorously as a series in n^{-1} , but numerical tests suggest that this does not give a significant advantage over Eq. (11).

Finally, when both a and z are short rational numbers, the binary splitting technique can be used to evaluate the continued fraction exactly (as a rational number). This would require $O(\ln n)$ multiplications of $O(n \ln n)$ -digit integers.

3 Convergence of Legendre's continued fraction

The continued fraction of Legendre can be rewritten similarly to Eq. (6),

$$e^z z^{1-a} \Gamma(a, z) = \frac{1}{1+} \frac{(1-a)v}{1+} \frac{v}{1+} \frac{(2-a)v}{1+} \frac{2v}{1+} \dots, \quad (12)$$

where $v \equiv z^{-1}$. The terms are $a_0 = 0$, $b_0 = 1$, $a_n = 1$, $b_{2n-1} = (n-a)v$, $b_{2n} = nv$ (for $n \geq 1$). This continued fraction converges for all z except real $z \leq 0$; however, the speed of convergence varies with z . Below I assume that a is not a positive integer (or else the continued fraction is finite).

Analytic estimates of the convergence rate of continued fractions are not often found in the literature. The estimate in Ref. [2] is partly heuristic and is only valid for real a . There is an analytic estimate for the continued fraction for Dawson's integral [14], but that estimate is based on a special property that does not hold for $\Gamma(a, z)$. Several general error estimates are available [15] but they require long computations. In this section I use the particular form of the Legendre continued fraction of Eq. (12) to obtain a direct *a priori* estimate of the required number of terms for a given absolute precision.

The forward recurrence

$$F_{0,n} - F_{0,n-1} = \frac{(-1)^n b_0 \dots b_{n-1}}{Q_n Q_{n+1}}, \quad (13)$$

where the sequence Q_n is defined by $Q_0 = 0$, $Q_1 = 1$, $Q_{n+2} = a_{n+1} Q_{n+1} + b_n Q_n$, gives an estimate for the convergence rate, provided that we have an asymptotic expression for the growth of Q_n . We shall use an analogous expression for the staggered convergents,

$$F_{0,n} - F_{0,n-2} = \frac{(-1)^{n-1} a_n b_0 \dots b_{n-2}}{Q_{n-1} Q_{n+1}}. \quad (14)$$

The sequence Q_n for the continued fraction of Eq. (12) is defined by

$$Q_{2n+2} = Q_{2n+1} + nvQ_{2n}, \quad (15)$$

$$Q_{2n+1} = Q_{2n} + (n-a)vQ_{2n-1}. \quad (16)$$

Equation (14) gives

$$F_{0,2n} - F_{0,2n-2} = -\frac{\Gamma(n-a)v^{2n-2}(n-1)!}{\Gamma(1-a)Q_{2n-1}Q_{2n+1}}.$$

We now need to estimate the asymptotic growth of Q_n . Since the recurrences for the odd and the even terms Q_n are different, we are motivated to consider a pair of generating functions

$$F(s) = \sum_{n=0}^{\infty} Q_{2n} \frac{s^n}{n!}, \quad G(s) = \sum_{n=0}^{\infty} Q_{2n+1} \frac{s^n}{n!}. \quad (17)$$

Using Eqs. (15)-(16), it is easy to show that

$$G = (1-vs) \frac{dF}{ds}, \quad \frac{dF}{ds} = (1-vs) \frac{dG}{ds} - (1-a)vG. \quad (18)$$

With the initial condition $G(0) = 1$, one obtains

$$G(s) = (1-vs)^{a-1} \exp\left[\frac{s}{1-vs}\right]. \quad (19)$$

The asymptotic behavior of Q_{2n-1} for large n can be found by the method of steepest descents (see e.g. [16]) on the contour integral around $s = 0$,

$$Q_{2n-1} = \frac{(n-1)!}{2\pi i} \oint_{(0)^+} G(s) s^{-n} ds. \quad (20)$$

The saddle points $s_{1,2}$ are found from the (quadratic) equation

$$\frac{dg}{ds} = -\frac{n}{s} - v \frac{a-1}{1-vs} + \frac{1}{(1-vs)^2} = 0, \quad (21)$$

where $g(s) \equiv \ln[G(s)s^{-n}]$. We are only interested in the leading asymptotic of the result for large n . The contribution of a saddle point s_i to Eq. (20) is

$$\frac{2\pi i Q_{2n-1}}{(n-1)!} \sim \frac{\sqrt{2\pi} e^{g(s_i)}}{\sqrt{-g''(s_i)}} = i\sqrt{\pi n} \frac{\exp\left(\pm 2\sqrt{nz} - \frac{z}{2}\right)}{z^n \left(\pm\sqrt{\frac{n}{z}}\right)^{a+\frac{3}{2}}} \left(1 + O\left(n^{-1/2}\right)\right). \quad (22)$$

We find (using the standard branch cut $Re\sqrt{z} \geq 0$) that the point s_1 (upper signs) gives the dominant contribution unless $Re\sqrt{v} = 0$. Then we obtain

$$|F_{0,2n} - F_{0,2n-2}| = \frac{4\pi \left|z^{\frac{3}{2}-a}\right| \sqrt{n}}{|\Gamma(1-a)|} \left|\exp(-4\sqrt{nz} + z)\right| \left(1 + O\left(n^{-1/2}\right)\right). \quad (23)$$

This asymptotic is valid for $n \gg |z|, |a|$. With our branch cut for \sqrt{z} ,

$$|\exp(-\sqrt{z})| = \exp\left(-\sqrt{\frac{|z| + \operatorname{Re} z}{2}}\right), \quad (24)$$

and it is clear that the sequence of Eq. (23) decays with n unless z is real and $z \leq 0$. The number of terms n needed to achieve an absolute precision $\varepsilon = 10^{-P}$ can be estimated from Eq. (23); one finds that n satisfies the equation

$$\sqrt{n} = \frac{P \ln 10 + \ln(4\pi\sqrt{n}) + \operatorname{Re} \left[z + \left(\frac{3}{2} - a\right) \ln z - \ln \Gamma(1 - a) \right]}{\sqrt{8(|z| + \operatorname{Re} z)}}. \quad (25)$$

To find n , it is enough to perform a few iterations of Eq. (25) starting with $n = 1$. It is clear that at fixed z one needs $2n = O(P^2)$ terms of the continued fraction for P digits of precision; the constant of proportionality depends on a and z . The required number of terms grows when z approaches the negative real semiaxis or zero, or when $\operatorname{Re} a > 0$ and $|a - 1| > e|z|$.

Numerical tests show that the estimate of Eq. (11),

$$F_{2n,\infty} \approx \frac{1}{2} \left(1 + \frac{a-1}{z} + \sqrt{\frac{4n}{z} + \left(1 - \frac{a-1}{z}\right)^2} \right), \quad (26)$$

gives a good approximation to the infinite remainder $F_{2n,\infty}$ of the continued fraction of Eq. (12) for large n . Use of this estimate improves the resulting precision by a few orders of magnitude but the convergence rate is unchanged.

The same analysis holds for the continued fraction of Eq. (6) which is a special case of Eq. (12) with $a = 1/2$.

4 Comparison of methods

4.1 Convergence of the Taylor series

Both series of Eq. (2) converge for all a and z (except when a is a negative integer), but their convergence and round-off behavior are not uniform. The series are not efficient when a is equal or close to a negative integer because of a cancellation between $\Gamma(a)$ and some terms of the form $1/(a+n)$. In this case, the recurrence relation can be used [4].

Consider the first series of Eq. (2). The magnitude of the ratio of successive terms is $|z|/|a+n+1|$. If $\operatorname{Re}(a+1) > 0$ and $|a+1| > |z|$, or if $|\operatorname{Im} a| > |z|$, then $|z| < |a+n+1|$ for all n and the convergence is monotonic. In this case it is enough to take $O(P/\ln P)$ terms for a precision of P digits. Otherwise, the rapid convergence regime begins only after $n_0 = O(|z|)$ terms. More precisely, n_0 is the largest positive integer for which $|a+n_0| < |z|$; approximately,

$$n_0 \approx -\operatorname{Re} a + \sqrt{|z|^2 - (\operatorname{Im} a)^2}. \quad (27)$$

The sum of the first n_0 terms may involve cancellations (especially for $\text{Re } z < 0$), and the working precision may need to be increased by $O(P)$ digits. This will not change the asymptotic complexity of the calculation. Therefore, we may estimate the complexity of the first series by $O(P/\ln P) + O(|z|)$ long multiplications.

The second series of Eq. (2) is simpler to analyze. The convergence is monotonic when $|z| < 1$, while for $|z| > 1$ one needs $n_0 = O(|z|)$ additional terms until the rapid convergence is achieved. (Again, we assume that a is not close to a negative integer.) Unlike the first series, the largest cancellations occur with $\text{Re } z > 0$. We obtain the same asymptotic complexity of $O(P/\ln P) + O(|z|)$ long multiplications.

4.2 Convergence of the asymptotic series

The asymptotic series of Eq. (3) starts to diverge after the n_0 -th term,

$$n_0 \approx \text{Re } a + \sqrt{|z|^2 - (\text{Im } a)^2}, \quad (28)$$

when the ratio of the successive terms $|n - a|/|z|$ becomes large. Therefore, Eq. (3) can be used for calculation if $|a| < |z|$, or if $|\text{Im } a| < |z|$ and $\text{Re } a > 0$. The minimum absolute error of the series is of the order of the n_0 -th term,

$$\left| z^{a-1} e^{-z} \frac{\Gamma(a) z^{-n_0}}{\Gamma(a - n_0)} \right| \sim e^{-2n_0} \quad (29)$$

(assuming $|z| > |a|$). This error is below the required precision $\varepsilon = 10^{-P}$ when $2n_0 \sim 2|z| > P \ln 10$. The working precision needs to be increased by $O(P)$ digits. We find that the cost of computation for a precision P for $|z| \gg P$ is at most $O(P)$ multiplications.

4.3 Complexity of $\Gamma(a, z)$

It is usual that the series and the continued fraction methods have somewhat complementary domains of applicability. The series converge rapidly at small z , while the continued fraction is most efficient at $1 < |a| < |z|$ or when $\text{Re } a < 0$. Using the explicit estimates of Eqs. (25) and (27), one can find the best methods.

For the practically important case $\text{Re } z > 0$, one could choose the series method for $|z| < P$ (which requires at most $O(P)$ terms) and the continued fraction method for $|z| > P$ (using again $O(P^2/z) \sim O(P)$ terms) if $\text{Re } a < 0$ and $|a| < |z|$. The asymptotic series method is used for $|z| > P$, $\text{Re } a > 0$ and $|z| > |a|$. Thus, the computation of the incomplete Gamma function $\Gamma(a, z)$ for $\text{Re } z > 0$ requires $O(P)$ long multiplications uniformly in z .

As already noted in [2], the computation of $\Gamma(a, z)$ for $\text{Re } z < 0$ is more computationally intensive. At the moment, a uniform bound on complexity does not seem to be available, although at fixed z the complexity is $O(P)$ if any of the series of Eq. (2) is used.

4.4 Complexity of $\operatorname{erfc} x$

The complementary error function $\operatorname{erfc} x$ can be computed somewhat faster than $\Gamma(a, z)$ because the “rectangular” method can be applied to the series of Eq. (2), reducing their complexity to $O\left(\sqrt{P/\ln P} + O(|z|)\right)$ long multiplications (here $z = x^2$). If we use the series for real x such that $|x| < O(P^{2/3})$ and the continued fraction for larger $|x|$, the overall complexity becomes $O(P^{2/3})$ uniformly in x .

4.5 Rational arguments

If both a and z are “short” rational numbers with $O(1)$ digits in the numerators and the denominators, the binary splitting technique can be used for the series as well as for the continued fraction computations (see Appendix). The complexity of the binary splitting method at very high precision can be estimated as $O(\ln P)$ multiplications of $O(P \ln P)$ -digit integers. As before, this estimate is uniform in the argument z if $\operatorname{Re} z > 0$.

A The binary splitting technique for continued fractions

If a continued fraction

$$F_{0,n} = a_0 + \frac{b_0}{a_1 +} \frac{b_1}{a_2 +} \dots \frac{b_{n-2}}{a_{n-1} +} \frac{b_{n-1}}{a_n} \quad (30)$$

contains only “short” terms, i.e. a_n and b_n are $O(\ln n)$ -digit integers or rationals, then the binary splitting technique can be applied to the computation of $F_{0,n}$. Here we sketch the algorithm and show that its complexity is equivalent to $O(\ln n)$ multiplications of $O(n \ln n)$ -digit integers.

Consider Eq. (30) as a function of $a_n \equiv p_n/q_n$, and compute the coefficients $A(0, n)$, $B(0, n)$, $C(0, n)$, $D(0, n)$ of the equivalent projective transformation for (p_n, q_n) :

$$F_{0,n} = \frac{A(0, n-1) a_n + B(0, n-1)}{C(0, n-1) a_n + D(0, n-1)} = \frac{A(0, n-1) p_n + B(0, n-1) q_n}{C(0, n-1) p_n + D(0, n-1) q_n}. \quad (31)$$

When we compute these coefficients as exact integers, we would only need to substitute the desired value for a_n to find $F_{0,n}$.

The coefficients A, B, C, D are computed for the subintervals $(0, n' - 1)$ and $(n', n - 1)$ recursively, using the matrix product of projective transformations,

$$T \equiv \begin{pmatrix} A & B \\ C & D \end{pmatrix}; \quad T(0, n-1) = T(0, n'-1) T(n', n-1). \quad (32)$$

Each time n' is chosen near the middle of the interval $(0, n - 1)$. At the base of recursion,

$$T(k, k) = \begin{pmatrix} a_k & b_k \\ 1 & 0 \end{pmatrix}. \quad (33)$$

The complexity of this method can be found as follows. The depth of the recursion is $O(\ln n)$ and there are 2^k matrix multiplications at level k . The elements of the matrix $T(l, m)$ have $O((m - l) \ln m)$ digits, and therefore the matrices at level k have elements with $O(n2^{-k} \ln n)$ digits. Since a multiplication is at least linear in the number of digits, 2^k multiplications with $n2^{-k}$ digits are faster than one multiplication with n digits. Therefore the total number of equivalent $O(n \ln n)$ -digit multiplications is equal to the recursion depth $O(\ln n)$.

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