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Note

The Determination of Incomplete Gamma Functions Through Analytic Integration

1. Introduction

In a recent note [6] it was shown that accurate values of the exponential integral

$$E_n(x) = \int_1^\infty e^{-xt} t^{-n} \, dt \tag{1}$$

can be obtained in the case of $E_1(x)$ thru a recursive procedure in the argument which will be termed *analytic integration.* The occurrence of these functions in the reduction of multi-center integrals is well known [5].

In order to establish the algorithmic reliability of analytic integration for our functions we shall discuss a remarkable error cancellation phenomenon. We shall consider the more general class of *incomplete gamma functions* defined by

$$\varphi(s, x) = e^x \int_1^\infty e^{-xt} t^{s-1} \, dt \tag{2}$$

where $\mathrm{Re}(x) > 0$. When n is a positive integer then one has $E_n(x) = e^{-x}\varphi(-n+1, x)$. One has the expansion

$$\varphi(s, x-h) = e^{-h}(\varphi(s, x) + h\varphi(s+1, x) + h^2\varphi(s+2, x)/2! + \cdots). \tag{3}$$

The convergence of this series will be examined later. The relation $\varphi(s+1, x) = (1 + s\varphi(s, x))/x$ allows one to introduce affine linear operators $T_1, T_2, T_3, \ldots$ by setting $T_n(\omega) = (1 + (s+n-1)\,\omega)/x$. One thus has $T_n T_{n-1} \cdots T_1(\varphi(s, x)) = \varphi(s+n, x)$.

We set $y = x + h$ and define the operator series

$$T_{x,y} = e^{-h}\left(I + hT_1 + \frac{h^2}{2!} T_1 T_2 + \cdots\right) \tag{4}$$

to obtain a transition operator with the property that $T_{x,y}(\varphi(s, x)) = \varphi(s, y)$. It is thus appropriate to call $T_{x,y}$ the *analytic continuation operator* relating $\varphi(s, x)$ and $\varphi(s, y)$.

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Qualitative description of the main results

(1) The series which defines the continuation operator converges if $|h/x| < 1$, where $h = x - y$.

(2) When all the variables are real then $T_{x,y}$ is error correcting when all the variables are real and $y < x$.

The continuation operator method has high precision for the entire range of real parameters s, whether negative or positive, and all positive arguments x. The method is especially attractive whenever there is need for multiple evaluations of $\varphi(s, x)$ with fixed parameter s and variable argument x.

In computer programs it was expedient to evalaute the modified series $T_{x,y} = e^{-h}(I + cS_1 + c^2S_2S_1 + \cdots)$ where $c = (x - y)/x$ and $S_n = M_n^{-1}T_nM_{n-1}$ with $M_n(\omega) = \omega x^n/n!$. Programs in ALGOL are available on request.

2. Analysis of the Continuation Operator

Let T be a function on an open complex domain D. When $T(\omega)$ is not zero then the formula $T(\omega(1 + \epsilon)) = T(\omega)(1 + \theta\epsilon)$ defines a number $\theta = \theta(\omega)$ which is called the *stability factor* of T at ω. When T is affine linear then $\theta = \omega T'(\omega)/T(\omega) = (T(\omega(1 + \epsilon)) - T(\omega))/T(\omega)\,\epsilon$. If $|\theta(\omega)| < 1$ then T is said to be *error correcting* at ω and if $|\theta(\omega)| > 1$ then T is said to be *error mangifying* at ω.

If S and T are two differentiable functions such that $T(\omega)$ and $ST(\omega)$ are distinct from zero then one has the *chain rule* $\theta_{ST}(\omega) = \theta_S(T\omega)\,\theta_T(\omega)$.

Example 2.1. We shall give a quantitative description of the instability which occurs in the recursive generation of incomplete gamme functions. Let $T = T_nT_{n-1} \cdots T_1$. One has $T(\varphi(s, x)) = \varphi(s + n, x)$ and thus our recursion proceeds in reverse to the direction considered in [6]. One has $\theta_{T^{-1}}(\omega) = \theta_T(\omega)^{-1}$ and thus our stability picture in comparison with that example is also reversed.

Use of the chain rule leads to the formula

$$\theta_T(\varphi(s, x)) = \varphi(s, x)\,\varphi(s + n, x)^{-1}\,x^{-n}\,s(s + 1)\cdots(s + n - 1) \tag{5}$$

The continued fraction appearing in [4] allows one to write $\varphi(s, x) = 1/(x + \omega(1 - s)/(\omega + 1))$. On the assumption that x is positive and s is real one has $\omega > 0$. When $s < 1$ one thus has the estimate $(x + 1)^{-1} < \varphi(s, x) < x^{-1}$.

One now deduces the easy estimate

$$|\theta_T(\varphi(-n, x))| \geqslant n!x^{-n}. \tag{6}$$

Take $x = 1$. When the residual error in computer representation of numbers is of relative magnitude 10^{-11} then a choice of $n = 15$ will suffice to guarantee total uncertainty of all digits in the computed number $T(\varphi(-n, x))$.

When $a = \operatorname{Re}(s)$ is positive then one has the estimate $|\varphi(s, x)| \leqslant e^u |x|^{-a} \Gamma(a)$, where $u = \operatorname{Re}(x)$. When $a + n$ is positive one thus has the estimate

$$\Big| \sum_{k \geqslant n} h^k \varphi(s + k, x)/k! \Big| \leqslant e^u |x|^{-a} \sum_{k \geqslant n} |c|^k \Gamma(a + k)/k! \tag{7}$$

where $c = h/x$ and $h = x - y$. When $|c| < 1$ the operator series (4) thus converges at the point $\varphi(s, x)$.

THEOREM 2.2. *The operator series*

$$T_{x,y} = e^{-h} \left(I + hT_1 + \frac{h^2}{2!} T_2 T_1 + \cdots \right),$$

where $h = x - y$, converges at every point when $|h/x| < 1$.

Proof. It suffices to demonstrate that the operator series converges at $\omega(1 + \epsilon)$ where ω is a point where the series is known to converge. Let $H_n = T_n T_{n-1} \cdots T_1$. We shall now consider

$$S = h^n H_n/n! + h^{n+1} H_{n+1}/(n + 1)! + \cdots + h^{n+m} H_{n+m}/(n + m)!.$$

In the estimate $|S(\omega(1 + \epsilon))| \leqslant |S(\omega)| + |S(\omega(1 + \epsilon)) - S(\omega)|$ the quantity $S(\omega)$ is a portion of a convergent series. Moreover, one has that

$$S(\omega(1 + \epsilon)) - S(\omega) = \sum_{k=n}^{n+m} (-c)^k \binom{-s}{k}, \tag{8}$$

where $c = h/x$. This sum is a portion of the expansion of $(1 - c)^{-s}$. It follows that our operator series converges at every point.

THEOREM 2.3. *If $|h/x| < 1$ then the stability factor of the continuation operator $T_{x,y}$ at $\omega = \varphi(s, x)$ is given by*

$$\theta(x, y) = e^{-h} \varphi(s, x)\, \varphi(s, y)^{-1} (y/x)^{-s} \tag{9}$$

where $h = x - y$.

Proof. Let $S = T_{x,y}$. One obtains from (8) that

$$S(\omega(1 + \epsilon)) - S(\omega) = e^{-h} \left(1 - \binom{-s}{1} c + \binom{-s}{2} c^2 \pm \cdots \right) \omega e = e^{-h} (y/x)^{-s}\, \omega \epsilon. \tag{10}$$

3. Extension of the Continuation Operators

We shall extend the operator $T_{x,y}$ to arbitrary positive real values x and y and we shall evade some technicalities found in the complex case.

Definition 3.1. If $T_{x,z}$ and $T_{z,y}$ satisfy $|(x-z)/x| < 1$ and $|(z-y)/z| < 1$ then one can set $T_{x,y} = T_{z,y}T_{x,z}$ provided $T_{x,y}$ is independent of z. An operator $T_{x,y}$ defined thus thru an arbitrary finite composition with the original operators will be called an *extended continuation operator* with arguments x and y.

Theorem 3.2. *The extended continuation operator $T_{x,y}$ with positive real arguments is independent of the decomposition used to define it. These operators satisfy the transitivity relations*

$$T_{x,y} = T_{z,y}T_{x,z}\,. \tag{11}$$

At $\varphi(s, x)$ the operator $T_{x,y}$ has the stability factor

$$\theta(x, y) = e^{-h}\varphi(s, x)\,\varphi(s, y)^{-1}(y/x)^{-s}. \tag{12}$$

Proof. Let $S = S_nS_{n-1}\cdots S_1$ and $T = T_mT_{m-1}\cdots T_1$ denote two decompositions corresponding to the interval determined by x and y in terms of the original operators so that $S(\varphi(s, x)) = T(\varphi(s, x)) = \varphi(s, y)$.

The chain rule, formula (9), and collapsing multiplication yield that $\theta(x, y) = e^{-h}\varphi(s, x)\,\varphi(s, y)^{-1}(y/x)^{-s}$ is the stability factor for both S and T at $\omega = \varphi(s, x)$. One has

$$S(\omega(1+\epsilon)) = S(\omega)(1+\theta(x, y)\,\epsilon) = T(\omega)(1+\theta(x, y)\,\epsilon) = T(\omega(1+\epsilon)). \tag{13}$$

Thru variation of ϵ one obtains that $S = T$ at every point. The general transitivity property is also immediate.

Remarks on the case of complex arguments. The uniqueness in the above theorem depends on the uniqueness of the value $\varphi(s, x)$ for real positive x. In the complex case the extended operators $T_{x,y}$ will depend on the paths chosen on a Riemann surface. Moreover, the transitivity property will not hold in general.

Corollary 3.3. *If s is a real parameter and $0 < y \leqslant x$ then the continuation operator $T_{x,y}$ is error correcting.*

Proof. One evaluates to find that

$$\begin{aligned}\theta(x, y) &= e^{-h}\varphi(s, x)\,\varphi(s, y)^{-1}(y/x)^{-s}\\ &= \int_x^\infty e^{-t}t^{s-1}\,dt \Big/ \int_y^\infty e^{-t}t^{s-1}\,dt < 1.\end{aligned} \tag{14}$$

4. The Remarkable Error Cancellation Phenomenon

W have already demonstrated that most terms in the computed series $e^{-h}(\omega + hT_1(\omega) + h^2T^2T_1(\omega)/2! + \cdots)$ can loose all numerical significance due to recursion error. What is remarkable is that the sum of such terms can be correct. This phenomenon is in part explained thru a calculation. For $H_n = h^nT_nT_{n-1} \cdots T_1/n!$ one has $H_n(\omega(1+\epsilon)) - H_n(\omega) = (-c)^n\binom{-s}{n}\,\omega\epsilon$. When $s < 0$ these terms may be large; however, their sum $(1-c)^{-s}\,\omega\epsilon$ is small.

Introduction of error into the series at a later stage leads to a generalization of our stability formula

$$R = e^{-h}(h^mI/m! + h^{m+1}T_{m+1}/(m+1)! + h^{m+2}T_{m+2}T_{m+1}/(m+2)! + \cdots) \quad (15)$$

$$S = e^{-h}(I + hT_1 + \cdots + h^{m-1}T_{m-1}T_{m-2} \cdots T_1/(m-1)!) \quad (16)$$

allows us to define $U(\alpha) = S(\omega) + R(\alpha)$. When $\omega = \varphi(s, x)$ and $\alpha = \varphi(s+m, x)$ then $U(\alpha) = \varphi(s, y)$ and one has the fomula

$$\theta_U(\alpha) = e^{-h}\varphi(s+m, x)\,\varphi(s, y)^{-1}\,F(s+m, 1, m+1, c)\,h^m/m! \quad (17)$$

where $F(s + , 1, m+1, c) = 1 + c(s+m)/(m+1) + c^2(s+m)(s+m+1)/(m+1)(m+2) + \cdots$ is a Gauss hypergoemetric series. In the absence of a generalization of (14) it is nevertheless possible to check that $\theta_U(\alpha)$ is small (when $\varphi(s, y)$ is computed from $\varphi(s, r)$ with $0 \leqslant y \leqslant x$) by making an actual evaluation of $\theta_U(\alpha)$.

5. Numerical Examples

Let truncated versions of (3) and (4) be denoted by

$$s_n = e^{-h}(\varphi(s, x) + h\varphi(s+1, x) + \cdots + h^n\varphi(s+n, x)/n!) \quad (18)$$

$$r_n = e^{-h}(I + hT_1 + \cdots + h^nT_nT_{n-1} \cdots T_1/n!)(\varphi(s, x)). \quad (19)$$

Examination of the stability formulas (12) and (17) shows that one can expect to produce numerical evidence of error cancellation only when s is negative and x is small. The table below came from a computer experiment where the arithmetic was accurate to eleven decimal digits.

TABLE I

n	r_n	s_n	$(s_n - r_n)/s_n$	
1	1.4105328406	1.4105328407	3.2(−11)	
6	1.7834376109	1.7834372653	−1.9(−7)	$x = 1/2$
11	1.7834219945	1.7834398441	1.0(−5)	$y = 1/16$
16	1.7834674305	1.7834398441	−1.6(−5)	$s = -31.5$
21	1.7834381685	1.7834398441	9.4(−7)	
26	1.7834398464	1.7834398441	−1.3(−9)	
31	1.7834398441	1.7834398441	2.6(−11)	
1	1.3098199998	1.3098199998	0	
6	8.2957465419	8.2957465418	−1.4(−11)	
11	1.6593509080	1.6593509080	−7.0(−12)	$x = 20$
16	1.7377817091	1.7377817092	−6.7(−12)	$y = 20 \cdot 2/3$
21	1.7390682648	1.7390682648	−6.7(−12)	$s = -31.5$
26	1.7390738449	1.7390838448	−6.7(−12)	
31	1.7390738533	1.7390738533	−6.7(−12)	

TABLE II

$\omega = \varphi(s, x) = 1.7937683115(-1)$		$s = -2$
$T_{x,y}(\omega) = \alpha = 4.7689685759(-1)$	$\theta(x, y) = 10^{-6}$	$x = 3$
$T_{y,x}(\alpha) = \omega = 1.7937683\underline{459}(-1)$	$\theta(y, x) = 10^{6}$	$y = 3(3/4)^{11}$

References

1. M. Abramowitz and T. Stegun, "Handbook of Mathematical Functions," Dover, New York, 1965.
2. W. Gautschi, Exponential integrals, *Comm. ACM* **16** (1973) 761–763.
3. N. Lebedev, "Special Functions and their Applications," Dover, New York, 1972.
4. O. Perron, "Die Lehre von den Kettenbruechen," Teubner, Stuttgart, 1957.
5. K. Rudenberg *et al.*, Study of two-center integrals ..., *J. Chem. Phys.* **24** (1956), 201–220.
6. R. Sharma and B. Zohuri, A general method for an accurate evaluation of exponential integrals $E_1(x)$, $x > 0$, *J. Comp. Phys.* **25** (1977), 199–204.
7. I. Stegun and R. Zucker, Automatic computing methods for special functions. II. The exponential integral $E_n(x)$, *J. Res. Nat. Bur. Standards Ser. B* **78** (1974), 199–216.
8. "Tables of Sine, Cosine and Exponential Integrals," Vols. I, II, U. S. Nat. Bur. Standards, 1940.

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