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Note

Reliable Evaluation of Gaussian Integrals

1. INTRODUCTION

A number of recent articles [2, 6, 7] appeal to the rapid evaluation of the Gaussian integrals

$$F_m(T) = \int_0^1 e^{-Tu^2} u^{2m}\, du \tag{1}$$

with T positive and $m = 0, 1, 2,\ldots$ in order to effect the evaluation of quantum-mechanical integrals.

In this note we shall discuss several aspects of the evaluation of the generalized Gaussian integrals

$$\alpha(s, x) = e^x \int_0^1 e^{-xt} t^{s-1}\, dt, \tag{2}$$

where $\mathrm{Re}(s) > 0$. The recursive relation $\alpha(s, x) = (x\alpha(s+1, x) + 1)/s$ enables one to continue the function to all complex numbers s save for the negative integers and zero. The restriction of this function to real parameters will be the concern of this note. The two functions that were introduced are related through the formula $F_m(T) = \frac{1}{2}e^{-T}\alpha(m + \frac{1}{2}, T)$. With respect to the incomplete gamma function $\gamma(s, x)$ in [1] one has $\alpha(s, x) = e^x x^{-s} \gamma(s, x)$.

In almost every occurrence, the function $\alpha(s, x)$ manifests itself for integral or half-integral parameters, but there occur notable exceptions. In [5] one encounters the need to evaluate integrals of the form

$$I(\mu, x) = \int_0^{(\mu-1)/2} e^{-xt} t^{1-\mu} (1 + t)^{1+\mu}\, dt \tag{3}$$

for $1 < \mu < 2$. The expansion

$$I(\mu, x) = f(\mu, x) \Big(\alpha(2 - \mu, \tfrac{1}{2}x(\mu - 1)) + \binom{1+\mu}{1} (\tfrac{1}{2}(\mu - 1))\, \alpha(3 - \mu, \tfrac{1}{2}x(\mu - 1))$$
$$+ \binom{1+\mu}{2} (\tfrac{1}{2}(\mu - 1))^2\, \alpha(4 - \mu, \tfrac{1}{2}x(\mu - 1)) + \cdots \Big), \tag{4}$$

where $f(\mu, x) = (\frac{1}{2}(\mu - 1))^{2-\mu} e^{-x(\mu-1)/2}$, enables one to evaluate $I(\mu, x)$ and effects a desired analytic continuation to the region $1 < \mu < 3$ save for $\mu = 2$.

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With respect to the formulas of Boys [2] the introduction of $\alpha(s, x)$ does not, in general, increase the complexity of evaluation of quantum-mechanical integrals, for the added exponential can be absorbed. Thus, for example, the electron repulsin integral [2, 3] may be written in the form

$$[aAbB \mid r_{21}^{-1} \mid cCdD] = \pi^{5/2} \frac{\alpha(1/2, T)}{(a+b)(c+d)(a+b+c+d)^{1/2}}$$
$$\exp\left(\frac{-ab}{a+b} \mid A - B \mid^2 + \frac{-cd}{c+d} \mid C - D \mid^2 - T\right),$$

where $T = (a+b)(c+d) \mid P - Q \mid^2/(a+b+c+d)$, $P = (aA+bB)/(a+b)$, and $Q = (cC+dD)/(c+d)$. A similar change in formulas can be made in [6].

2. Computation through Backwards Recursion

The recursive relation $\alpha(s, x) = (x\alpha(s+1, x)+1)/s$ motivates the introduction of sequences of affine linear operators $S_1, S_2, S_3,\ldots$ through $S_n(\omega) = (x\omega + 1)/(s+n-1)$. One has $S_n(\alpha(s+n, x)) = \alpha(s+n-1, x)$ and $S_1 S_2 \cdots S_n(\alpha(s+n, x)) = \alpha(s, x)$. It is understood that there is a dependence of the operators on a fixed parameter s and a fixed argument x. If $S = S_1 S_2 \cdots S_n$, then one has

$$S(0) = \frac{1}{s} + \frac{x}{s(s+1)} + \cdots + \frac{x^{n-1}}{s(s+1)\cdots(s+n-1)} \tag{5}$$

which is a truncation of the infinite series [1, 7]

$$\alpha(s, x) = \frac{1}{s} + \frac{x}{s(s+1)} + \frac{x^2}{s(s+1)(s+2)} + \cdots. \tag{6}$$

The operator notation has both algorithmic and analytic utility. Let $T(\omega) = a\omega + b$ be an affine linear function. When $T(\omega)$ is not zero, then the formula

$$T(\omega(1+\epsilon)) = T(\omega)(1 + \theta_T(\omega)\epsilon) \tag{7}$$

defines $\theta_T(\omega) = (T(\omega(1+\epsilon)) - T(\omega))/T(\omega)\epsilon$, a quantity which shall be termed the *stability factor* of T at ω. One has that $\theta(\omega) = \theta_T(\omega) = \omega T'(\omega)/T(\omega)$. This formula extends the definition of the stability factor to differentiable functions. If $\mid \theta(\omega)\mid < 1$, then T will be said to be *error correcting* at ω. If S and T are two differentiable functions such that $T(\omega)$ and $ST(\omega)$ are different from zero, then one has the *chain rule* $\theta_{ST}(\omega) = \theta_S(T\omega)\,\theta_T(\omega)$.

THEOREM 2.1. *If $S = S_1 S_2 \cdots S_n$, then the stability factor of S at $\omega = \alpha(s+n, x)$ is given by*

$$\theta_S(\omega) = x^n \frac{\Gamma(s)}{\Gamma(s+n)} \alpha(s+n, x)\, \alpha(s, x)^{-1}. \tag{8}$$

The stability factor satisfies the estimate

$$0 \leqslant \theta_S(\omega) \leqslant \min\{x^{n-m}\Gamma(m)/\Gamma(n) \mid 0 < m \leqslant n\}. \tag{9}$$

The stability factor is related to relative truncation error through the relation

$$S(0) = \alpha(s, x)(1 - \theta_S(\omega)). \tag{10}$$

Estimate (9) is in actual fact a relative truncation error estimate and is similar to the absolute error estimate in [8].

A useful estimate for $\alpha(s, x)$ is

$$1/s < \alpha(s, x) < 1/(s - x), \tag{11}$$

which is valid whenever $s > x > 0$.

Let $n(s, x)$ denote the smallest index so that the truncation (5) approximates $\alpha(s, x)$ to eleven decimal digits. This index function may be computed from (8) or (9). A tabulation of $n(s, x)$ is made in Table I.

Methods of evaluation. Several methods exist for evaluating the truncated series and the backwards iterates. There is no mention in the literature of the second method.

I. Through the help of the formula $s/x = (s - 1)/x + 1/x$ it is possible to make a forward evaluation of (5) in $[n(x) + 1]$ operations, where $n(x)$ denotes the truncation index.

II. In backwards recursion one may evaluate the recursive transformations in pairs through exploitation of additive relation in a manner which requires only one division. As a result $S(0)$, corresponding to (5), may be evaluated in $[\frac{1}{2}(n(x) + 5)]$ operations.

In backwards evaluation it is expedient to approximate the starting index through linearizations. For example, $n(x) = 15 + [4(x - 1)]$ $(1 \leqslant x \leqslant 5)$ and $n(x) = 30 + [2(x - 5)]$ $(5 \leqslant x \leqslant 10)$ approximate well the starting indices $n(1/2, x)$ in Table I.

TABLE I

x	$n(1/2, x)$	$n(33/2, x)$	x	$n(1/2, x)$	$n(33/2, x)$
1	15	8	6	31	16
2	19	10	7	34	18
3	23	12	8	36	20
4	26	13	9	38	21
5	29	15	10	40	23

EXAMPLE 2.2. Backwards recursion is particularly suitable to the evaluation of series (4). One obtains from (3) the operator

$$T = f(\mu, x)$$

$$\left(S_1 \cdots S_n + \binom{1+\mu}{1} (\tfrac{1}{2}(\mu - 1)) S_2 \cdots S_n + \cdots + \binom{1+\mu}{n} (\tfrac{1}{2}(\mu - 1))^n S_n\right). \quad (12)$$

One has $T(\alpha(3 + n - \mu, \frac{1}{2}x(\mu - 1) = I(\mu, x) + O((\mu - 1)/2)^n)$.

3. COMPUTATION THROUGH TAYLOR EXPANSION

The process of computing function values through Taylor expansions has been quite useful and may be the most rapid method for generating the functions under consideration [4]. However, the computation of $\alpha(s, x + h)$ from $\alpha(s, x)$ through series expansions in which the coefficients are recursively generated allows one to adopt an operator point of view [9]. From the numerical perspective the behavior of our operator series is somewhat distinct from the behavior of series with exactly determined coefficients.

One has the expansion

$$\alpha(s, x + h) = e^h(\alpha(s, x) - h\alpha(s + 1, x) + h^2\alpha(s + 2, x)/2! \pm \cdots). \quad (13)$$

Let T_1, T_2, T_3,... be affine linear operators defined by $T_n(\omega) = ((s + n - 1)\omega - 1)/x$. One has that $T_n(\alpha(s + n - 1, x)) = \alpha(s + n, x)$ and $T_n T_{n-1} \cdots T_1(\alpha(s, x)) = \alpha(s + n, x)$. If one sets

$$T_{x,y} = e^h(I - hT_1 + h^2T_2T_1! \pm \cdots), \quad (14)$$

where $h = y - x$, then one obtains a *continuation operator* with the property that $T_{x,y}(\alpha(s, x)) = \alpha(s, y)$.

If $T = T_nT_{n-1} \cdots T_1$ and $S = S_1S_2 \cdots S_n$, then $T = S^{-1}$ and one has the formula $\theta_T(\alpha(s, x)) = \theta_S(\alpha(s + n, x))^{-1}$, which expresses the fact that T is unstable to the same degree that S is stable. Thus (14) is a series of unstable operators. In [9] we established an *error cancellation* principle for a similar series. An analogous computation can be made here. For $H_n = h^nT_nT_{n-1} \cdots T_1/n!$ one has the formula

$$H_n(\omega(1 + \epsilon)) - H_n(\omega) = c^n \binom{-s}{n} \omega\epsilon, \quad (15)$$

where $c = h/x$. Upon summation one obtains

$$T_{x,y}(\omega(1 + \epsilon)) - T_{x,y}(\omega) = (1 + c)^{-s}\omega\epsilon = (y/x)^{-s}\omega\epsilon. \quad (16)$$

When $y > x$ and $s > 0$, then the above quantity is small, a fact which may be interpreted to mean that first-order errors propagate in such a manner that their sum is small. It is possible to write formulas which assert that errors introduced into the recursion process at a later stage also have the cancellation property.

THEOREM 3.1. *The operator series*

$$T_{x,y} = e^h(I - hT_1 + h^2T_2T_1/2! \pm \cdots),$$

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

THEOREM 3.2. *The stability factor* $\theta = \theta(x, y)$ *of* $T_{x,y}$ *at* $\alpha(s, x)$ *is given by the formula*

$$\begin{aligned}\theta(x, y) &= e^h\alpha(s, x)\,\alpha(s, y)^{-1}(y/x)^{-s} \\ &= \int_0^x e^{-t}t^{s-1}\,dt \Big/ \int_0^y e^{-t}t^{s-1}\,dt.\end{aligned} \tag{17}$$

Let $n(x, h)$ denote the index of truncation for the operator evaluation $T_{x,x+h}(\alpha(s, x)) = \alpha(s, x + h)$ so that at $\alpha(s, x)$ the operator $T_{x,x+h}$ is approximated by

$$e^h(I + hT_1 + h^2T_2T_1/2! + \cdots + (-h)^{n-1}T_{n-1} \cdots T_2T_1/(n-1)!) \tag{18}$$

to 11 significant digits [3]. A tabulation is made in Table II.

TABLE II

x	$n(x, 1)$	$n(x, 1/10)$	$(s = 1/2)$	$n(x, 1)$	$n(x, 1/10)$	$(s = 33/2)$
2	12–70	6		53–70	7	
5	11	6		14	7	
10	10	5		14	7	
20	7	4		13	7	
30	6	4		12	6	
40	6	4		11	6	

Method of evaluation. It is possible to effect the evaluation of (18) in $3n(x, h)$ operations. One writes $T_n(\omega) = ((s + n - 1)/x)\omega + 1/x$, which allows that the computation of $T_n(\omega)$ is one operation, for the coefficient can be updated through the addition of $1/x$. Similarly, $h^n/n!$ can be generated from $h^{n-1}/(n-1)!$ through division by a quantity which is updated through addition.

EXAMPLE 3.3 (A divergent operator series). Let T_1, T_2, T_3,... correspond to $\alpha(2 - \mu, \frac{1}{2}x(\mu - 1))$. Define

$$T = I + \binom{1+\mu}{1}(\tfrac{1}{2}(\mu - 1))\,T_1 + \binom{1+\mu}{2}(\tfrac{1}{2}(\mu - 1))^2\,T_2T_1 + \cdots. \tag{19}$$

One has the perturbation calculation

$$T(\omega(1+\epsilon)) - T(\omega)$$
$$= \omega\epsilon\left(1 + \binom{1+\mu}{1}\left(\frac{2-\mu}{x}\right) + \binom{1+\mu}{2}\left(\frac{2-\mu}{x}\right)\left(\frac{3-\mu}{x}\right) + \cdots\right),$$

which allows one to infer that T converges only at the ideal point $\alpha(2-\mu, \frac{1}{2}x(\mu-1))$. Since the perturbed series diverges quite fast, one cannot expect to evaluate (4) with forward recursion, save in an asymptotic manner.

Caution. While $T_{x,y}$ is error correcting for $y > x$, one should limit $h = y - x$ so that $|h| < 1$. This is necessary because (14) is an alternating series in the upward direction.

The error cancellation phenomenon has been tested on actual computers in the parameter range $0 \leqslant s \leqslant 20$ with $|c| \leqslant \frac{1}{2}$. However, the property may fail when s is large, x is small, and c is near unity.

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