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COMPUTING THE CONFLUENT HYPERGEOMETRIC FUNCTION, M(a,b,x)

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ABSTRACT

The confluent hypergeometric function, $M(a, b, x)$, arises naturally in both statistics and physics. Although analytically well-behaved, extreme but practically useful combinations of parameters create extreme computational difficulties. A brief review of known analytic and computational results highlights some difficult regions, including $b > a > 0$, with x much larger than b. Existing power series and integral representations may fail to converge numerically, while asymptotic series representations may diverge before achieving the accuracy desired. Continued fraction representations help somewhat. Variable precision can circumvent the problem, but with reductions in speed and convenience.

In some cases, known analytic properties allow transforming a difficult computation into an easier one. The combination of existing computational forms and transformations still leaves gaps. For $b > a > 0$, two new power series, in terms of Gamma and Beta cumulative distribution functions respectively, help in some cases. Numerical evaluations highlight the abilities and limitations of existing and new methods. Overall, a rational approximation due to Luke and the new Gamma-based series provide the best performance.

1. INTRODUCTION

1.1 Motivation

A very simple and practical need drove the work presented here. In general, only approximations are available for the power of a test of the general linear hypothesis in the general linear multivariate model (12). A method of moments approach holds the promise of improved approximations. In some cases, the expected value of the Pillai-Bartlett trace statistic (6) may be represented as a double infinite series. Accurate numerical evaluation of the series proves difficult, especially for small sample sizes with high power, conditions often of practical importance. One escape route was opened by the observation that the inner series may be expressed as a weighted sum of two confluent hypergeometric functions. However, in a wide range of important cases, the strategy merely replaced one computational difficulty with a similar one. A method for computing the confluent hypergeometric function was needed. To be conveniently useful, the method would 1) achieve accuracy to fixed machine precision of the computer software in use, 2) be robust to extreme combinations of inputs, and 3) use fixed precision. Computing speed would be less important than accuracy. Progressively more thorough searches of the literature and manipulations of published forms failed to find any collection of methods that succeeded.

The confluent hypergeometric function arises naturally in the study of certain random variables. For example, the density and characteristic function of the noncentral F have simple forms in terms of the function (5, Chapter 30). The function also contains other functions as special cases, including many that are widely used in mathematical physics (6, 8). Special cases include the Bessel functions, the incomplete gamma (and hence further special cases including, error functions and Fresnel integrals), Laguerre polynomials, Hermite polynomials, Coulomb wave functions, and parabolic cylinder functions. The confluent hypergeometric function represents a limiting special case of Gauss' hypergeometric function (1, Chapter 13; 8; 11, §5.2). In turn, mathematicians have considered generalized hypergeometric functions. The attention given to the function has helped create a wealth of information about its analytic properties, including power series representations, integral representations, and asymptotic approximations.

Less attention has been given to computing the function. With fixed precision arithmetic, computations with even reasonably sophisticated implementations of power series and integral representations fail completely for input ranges of practical importance. For the same inputs, asymptotic approximations sometimes diverge before achieving the desired accuracy.

1.2 Literature Review

Many authors discuss the confluent hypergeometric function briefly, while a few devote substantial coverage to it. Two sources stand out from the rest. Chapter 13 in (1) contains a very succinct and extensive summary of analytic properties. Slater's monograph (17) provides a thorough and very well-written treatment of the analytic properties of the function. Both include extensive bibliographies. More general functions, with vector or matrix rather than scalar inputs, have also attracted serious attention (10).

Dingle (3) provided an extensive treatment of asymptotic approximations in general. The index includes nineteen references to the confluent hypergeometric function. Following Dingle (page v), "the designation 'asymptotic' will be reserved for those series in which for large values of the variable at all phases the terms first progressively decrease in magnitude, then reach a minimum and thereafter increase." Hence such series ultimately diverge. Wider, and sometimes conflicting, interpretations occur elsewhere in statistics, mathematics, and physics. In contrast, for the purposes of this paper, a finite or infinite series will be considered analytically "exact" if, with variable precision arithmetic, the sum may be computed to any desired level of accuracy.

In principle, the confluent hypergeometric function may be computed as a power series, an integral of a function, or a solution to a differential equation. Only the first approach has received any significant attention for computations. Relph (15) described how to implement a simple power series representation. Luke (9) devoted a chapter to rational approximations of the function. Luke's approach involves a recurrence relation, based on polynomials involving third powers of the parameter. Brent (2) discussed using variable precision to achieve any desired level of accuracy in computing special functions. See van der Laan and Temme (20) for a general introduction to the calculation of special functions (especially Chapter I, an annotated bibliography, and Chapter II, a review of general aspects). Temme (18) discussed computing an independent solution to the differential equation, often indicated at $U(a, b, x)$. Thompson (19) provided a very appealing and contemporary treatment of the general area of computing special functions, including specific coverage of the confluent hypergeometric.

2. SOME KNOWN RESULTS AND IMPLICATIONS

2.1 Notation

For $\nu > 0$, write the Gamma function as

$$\Gamma(\nu) = \int_0^\infty e^{-t} t^{\nu-1} dt\,, \tag{2.1}$$

and the incomplete Gamma function as

$$\gamma(x;\nu) = \int_0^x e^{-t} t^{\nu-1} dt\,. \tag{2.2}$$

Write the cumulative distribution function (CDF) of a Gamma random variable as $F_\gamma(x;\nu) = \gamma(x;\nu)/\Gamma(\nu)$.

Define the factorial function for a positive integer, n, as

$$\begin{aligned} n! &= \prod_{k=1}^{n} k \\ &= \Gamma(n+1)\,. \end{aligned} \tag{2.3}$$

Define the ascending factorial, also referred to as Pochhammer's symbol, as

$$\begin{aligned} (a)_i &= \prod_{k=0}^{i-1}(a+k) \\ &= \frac{\Gamma(a+i)}{\Gamma(a)}\,, \end{aligned} \tag{2.4}$$

with $(a)_0 = 1$. If a a negative integer and $i \geq -a$, then $(a)_i = 0$. Also $(1)_n = n!$.

For the vectors $\boldsymbol{a}$ $(p \times 1)$ and $\boldsymbol{b}$ $(q \times 1)$, define the generalized hypergeometric function as

$${}_pF_q(\boldsymbol{a};\boldsymbol{b};x) = \sum_{i=0}^{\infty} \frac{\prod_{j_p=1}^{p} (a_{j_p})_i}{\prod_{j_q=1}^{q} (b_{j_q})_i} \frac{x^i}{i!}\,. \tag{2.5}$$

Write one solution to Kummer's equation (1) as:

$$\begin{aligned} M(a,b,x) &= \sum_{i=0}^{\infty} \frac{(a)_i}{(b)_i} \frac{x^i}{i!} \\ &= {}_1F_1(a;b;x)\,. \end{aligned} \tag{2.6}$$

Many different notations have been used. Various authors refer to either $M(a,b,x)$ or the independent solution $U(a,b,x)$ as the confluent hypergeometric function.

2.2 Some Properties of $M(a, b, x)$

Only real a, b, and x will be considered. The analytic and associated computational behavior of $M(a, b, x)$ splits into a number of distinct regions (1, §13.1.2, p504; 17, p113-116). If $a = 0$ or $x = 0$ then $M(a, b, x) = 1$. If neither a nor b are negative integers, then the series converges for all finite x. If a is a negative integer while b is not, the series terminates as a finite polynomial of order $|a|$ in x. The same result holds if $b - a$ is a negative integer while b is not, except for a factor of $\exp(x)$. Abramowitz and Stegun (1) listed twenty special cases that allow writing $M(a, b, x)$ in terms of other functions. For example, $M(a, a, x) = \exp(x)$ and $M(a, a + 1, -x) = ax^{-a}\gamma(x; a)$. One of the recurrence relations or differential properties may allow converting to one of the special cases.

One of Kummer's transformations has particular promise for computations:

$$M(a, b, x) = \exp(x) M(b - a, b, -x)\,. \tag{2.7}$$

However, for positive a and b, introducing the alternating sign may decrease numerical stability. The change represents what Lauwerier (7, p106) called "eulerization," the transformation of a power series to increase speed of convergence.

Abramowitz and Stegun (1, equation 13.2.1) give a useful integral form for $b > a > 0$:

$$M(a, b, x) = \frac{\Gamma(b)}{\Gamma(a)\Gamma(b-a)} \int_0^1 \exp(xt) t^{a-1} (1-t)^{b-a-1} dt\,. \tag{2.8}$$

A number of exact (infinite) series representations can be written in terms of various Bessel functions. For the cases examined here, such series give no advantage for computation.

2.3 Continued Fractions

For sequences $\{a_i\}$ and $\{b_i\}$, write a continued fraction as

$$C = b_0 + \cfrac{a_1}{b_1 + \cfrac{a_2}{b_2 + \cfrac{a_3}{b_3 + \cfrac{a_4}{b_4 + \ddots}}}}\,. \tag{2.9}$$

Jones and Thron (4) provided a comprehensive treatment from an analytic perspective. They described methods for creating continued fraction and Padé approximations. Press, Teukolsky, Vetterling, and Flannery (14, §5.1-5.2) discussed computing with continued fractions.

Direct evaluation of C involves backwards recursion, and hence complete recalculation to change the number of terms. For a three-term forward recurrence algorithm let $A_{-1} = 1$, $A_0 = b_0$, $B_{-1} = 0$, and $B_0 = 1$. Then for $i \geq 1$ write the i^{th} approximant as $M_i = A_i / B_i$, with

$$A_i = b_i A_{i-1} + a_i A_{i-2} \tag{2.10}$$

$$B_i = b_i B_{i-1} + a_i B_{i-2}\,. \tag{2.11}$$

Jones and Thron (4, p37) described Euler's (1748) method for converting an infinite series into a continued fraction. Consider the special case of a power series,

$$S = \sum_{i=0}^{\infty} x^i c_i \,, \tag{2.12}$$

with $c_i \neq 0$. Let $a_1 = c_1 x$ and $b_1 = 1$. For $i > 1$ define $r_i = c_i / c_{i-1}$, $a_i = -r_i x$ and $b_i = 1 + r_i x$. Also let $A_{-1} = 1$, $A_0 = c_0$, $B_{-1} = 0$, and $B_0 = 1$. In turn $A_1 = c_0 + c_1 x$, $B_1 = 1$, and $M_1 = c_0 + c_1 x$. For $i > 1$

$$\begin{aligned} A_i &= (1 + r_i x) A_{i-1} - r_i x A_{i-2} \\ &= A_{i-1} + r_i x A_{i-1} - r_i x A_{i-2} \\ &= A_{i-1} + r_i x (A_{i-1} - A_{i-2}) \,. \end{aligned} \tag{2.13}$$

A power series has $B_i \equiv 1$ for $i \geq 0$. Therefore, for $i > 1$, write $M_i = A_i$, with the last form having the most appeal for the application of interest.

Jones and Thron (4, p11, p26, and elsewhere) discussed algorithms for evaluating continued fractions, including the forward (FR) and backward (BR) recurrence algorithms. In their chapter on the analysis of the numerical stability of the BR algorithm they cited research "...which seems to indicate that the backward recurrence algorithm (BR algorithm) is numerically more stable than the FR algorithm." They followed this faint praise with similarly hedged discussions. The BR algorithm requires complete recalculation to change the number of terms used.

2.4 Computational Forms for $M(a, b, x)$

Method 1; Defining Power Series in x. Relph's (15) code for computing $M(a, b, x)$ uses the following steps. Define

$$M_I = \sum_{i=0}^{I} \frac{(a)_i}{(b)_i} \frac{x^i}{i!} \,. \tag{2.14}$$

Let $T_0 = 1$ and, for $i > 0$,

$$T_{i+1} = T_i \cdot \frac{(a+i)}{(b+i)} \frac{x}{(i+1)} \,. \tag{2.15}$$

Then $M_0 = 1$ and, for $i > 0$, use the recurrence relationship to compute

$$M_{i+1} = M_i + T_{i+1} \,. \tag{2.16}$$

The process stops with sufficiently small $|T_{i+1}/M_{i+1}|$ or, if $|M_{i+1}| \approx 0$, sufficiently small $|T_{i+1}|$. In some cases T_i increases in size before beginning to decrease. Thompson (19, §16.2, p463) also provided code for the method. He recommended using it if $|x| < 50$, and otherwise switching to an asymptotic approximation.

Method 1C; Continued Fraction for Defining Power Series in x. Write $A_{-1} = A_0 = 1$ and $A_1 = 1 + xa/b$. Also define, for $i > 1$, $r_i = (a + i - 1)/[i(b + i - 1)]$ and

$A_i = A_{i-1} + (A_{i-1} - A_{i-2})r_i x$. Let $M_0 = 1$. For $i > 1$ compute the i^{th} approximant to $M(a, b, x)$ as $M_i = A_i$.

Method 2; Asymptotic Series in x^{-1}. When applicable, asymptotic approximations may be numerically robust. Thompson (19, p466) wrote, for $b > a > 0$ and $|x| \gg 0$,

$$M(a, b, x) \asymp \exp(x)\frac{\Gamma(b)x^{a-b}}{\Gamma(a)}\sum_{i=0}^{I}\frac{(b-a)_i(1-a)_i}{i!x^i}, \tag{2.17}$$

$$M(a, b, -x) \asymp \frac{\Gamma(b)x^{-a}}{\Gamma(b-a)}\sum_{i=0}^{I}\frac{(1+a-b)_i(a)_i}{i!x^i}. \tag{2.18}$$

Convergence factors are available for these forms. For some combinations of (a, b, x) the approximations diverge before achieving the accuracy desired. Two examples are $M(100, 102, 10)$ and $M(4000, 4001, 4000)$. See Table 3 and the discussion surrounding Table 4 for more detail about these and other examples.

Method 2C; Continued Fraction for Asymptotic Series in x^{-1}. Let $A_{-1} = A_0 = 1$. If $x > 0$ let $A_1 = 1 + (b-a)(1-a)/x$ and $r_i = (b - a + i - 1)(i - a)/i$ for $i > 1$. If $x < 0$ let $A_1 = 1 + (1 + a - b)a/x$ and $r_i = (a - b - i)(a - i - 1)/i$. In either case: i) $A_i = A_{i-1} + (A_{i-1} - A_{i-2})r_i/x$, ii) $M_0 = 1$, and iii) for $i > 1$ compute the i^{th} approximant as $M_i = A_i$.

Method 3; A Rational Approximation (9, p182-183). If $x > 0$ let $\delta = (b-a)$, $Q_0 = 1$, $Q_1 = 1+x(\delta+1)/(2b)$, $Q_2 = 1+x(\delta+2)/[2(b+1)] + x^2(\delta+1)(\delta+2)/[12b(b+1)]$, $P_0 = 1$, $P_1 = Q_1 - x\delta/b$, and $P_2 = Q_2 - (x\delta/b)\{1+x(\delta+2)/[2(b+2)]\} + x^2\delta(\delta+1)/[2b(b+1)]$. Also

$$\begin{aligned} f_{i1} &= \frac{(i-\delta-2)}{2(2i-3)(i+b-1)} \\ f_{i2} &= \frac{(i+\delta)(i+\delta-1)(i-\delta-2)}{4(2i-1)(2i-3)(i+b-2)(i+b-1)} \\ f_{i3} &= -\frac{(i+\delta-2)(i+\delta-1)(i+\delta-2)}{8(2i-3)^2(2i-5)(i+b-3)(i+b-2)(i+b-1)} \\ f_{i4} &= -\frac{(i+\delta-1)(i-b-1)}{2(2i-3)(i+b-2)(i+b-1)}. \end{aligned} \tag{2.19}$$

For $i \geq 3$

$$P_i = (1 + f_{i1}x)A_{i-1} + (f_{i4} + f_{i2}x)A_{i-2} + f_{i3}x^3 A_{i-3} \tag{2.20}$$

and

$$Q_i = (1 + f_{i1}x)B_{i-1} + (f_{i4} + f_{i2}x)B_{i-2} + f_{i3}x^3 B_{i-3}. \tag{2.21}$$

Write the i^{th} approximant as $M_i = P_i/Q_i \approx \exp(-x)M(a, b, x) = M(b - a, b, -x)$.

3. SOME NUMERICAL EVALUATIONS

3.1 Methods

The problem that stimulated this work required computing $M(n/2+j, n/2+2j+1, x)$ for $x > 0$, $n \in \{3,4,5,\dots\}$ and $j \in \{0,1,2\dots\}$. Both x (a function of a noncentrality parameter) and n (a function of an error degrees of freedom) could be 1000 or larger. In such cases computing $\exp(x)M(j+1, n/2+2j+1, -x)$ seems preferable. Apparently the problem does not reduce to any convenient special case. All numerical examples were chosen to represent combinations of this nature. For the computations in this section attention was restricted to $0 < x \leq 5000$, $0 \leq j \leq 100$ and $3 \leq n \leq 5000$. Both $M(n/2+j, n/2+2j+1, x)$ and $\exp(x)M(j+1, n/2+2j+1, -x)$ were always computed.

All of the numerical work reported in this paper was conducted in SAS IML®(16), in SAS Version 6.12, running under OS/2®. The environment provides precision comparable to double precision in Fortran, with roughly 15 decimal digits of accuracy available. Each function declared convergence if the relative change was less than 10^{-10} in absolute value. Results were printed to five digits. In this first set of studies, all series were limited to 150 terms. Go to the web site http://www.bios.unc.edu/~muller to get free IML code and documentation.

3.2 Enumeration Results

Some enumerations for Methods 1-3 led to a number of conclusions. Computation with the power series (Method 1) worked well for small $|xa/b|$. Accuracy disappeared as $|x|$ increased (for a and b fixed). A continued fraction extended the range. At least for the examples discussed here, with fixed precision arithmetic, a forwards algorithm (Method 1C) allowed accurate calculation with the power series for somewhat larger values of $|xa/b|$ than did a backwards algorithm. The rational approximation (Method 3) extended the range much more. However, all formulations eventually failed for sufficiently large $|xa/b|$. The asymptotic expansions (Method 2) were numerically stable. However, as $|b|$ and $|x|$ both increase, not necessarily at the same rate, as may happen in the application of interest, then Method 2 sometimes diverged before achieving the accuracy desired. Numerical quadrature of the integral form was also tried. The approach was much slower than any other. Furthermore, both of two different and reasonably sophisticated quadrature methods failed to converge as $|xa/b|$ became large. See §5 for a more detailed analysis of the numerical performance of the various methods.

Slater (17) noted that if $a \approx b$ then $M(a,b,x) \approx \exp(x)$. Method 5 implies that $M(a,b,x) \approx \exp(xa/b)$ provides a first-order approximation, which implies that, as a rough approximation, the numerical behavior of $M(a,b,x)$ depends on $|xa/b|$. Examination of the results in this section led to the conclusion that large values of the $i = 1$ term predicts difficulty with any of the algorithms. Hence for Methods 1, 1C, and perhaps Method 3, examine $|xa/b|$. For Methods 2 and 2C, examine $|(b-a)(1-a)/x|$ if $x > 0$ and $|(1+a-b)a/(-x)|$ if $x < 0$.

4. NEW METHODS FOR COMPUTING $M(a,b,x)$

4.1 A New Expansion in Terms of the Incomplete Gamma Function

Method 4; Exact Power Series in x^{-1} and Gamma's. If $b > a > 0$ and $x > 0$, then write

$$M(a,b,-x) = \frac{\Gamma(b)}{\Gamma(a)\Gamma(b-a)} \int_0^1 \exp(-xt) t^{a-1} (1-t)^{b-a-1} dt\,. \tag{4.1}$$

With $f(t) = (1-t)^{b-a-1}$, use the (generalized) binomial theorem to write a Taylor's series expansion for $f(t)$ about the point $t_0 = 0$ as

$$\begin{aligned} f(t) &= \sum_{i=0}^{\infty} \frac{(t-t_0)^i}{i!} f^{(i)}(t_0) \\ &= \sum_{i=0}^{\infty} (a-b+1)_i \frac{t^i}{i!}\,. \end{aligned} \tag{4.2}$$

Substituting this expansion into the integral form yields (for $b > a > 0$, and $x > 0$)

$$\begin{aligned} M(a,b,-x) &= \frac{\Gamma(b)}{\Gamma(b-a)\Gamma(a)} \int_0^1 \exp(-xt) \sum_{i=0}^{\infty} (a-b+1)_i \frac{1}{i!} t^{i+a-1} dt \\ &= \frac{\Gamma(b)}{\Gamma(b-a)\Gamma(a)} \sum_{i=0}^{\infty} (a-b+1)_i \frac{1}{i!} \int_0^1 \exp(-xt) t^{i+a-1} dt\,. \end{aligned} \tag{4.3}$$

The validity of the exchange of integration and summation reduces to two cases. For integer $(b-a)$ (positive by assumption) the sum terminates finitely at $i = (b-a)$. Otherwise let n indicate the largest integer with $n > |a-b+1|$. Then

$$\begin{aligned} \sum_{i=0}^{\infty} (a-b+1)_i \frac{t^i}{i!} &= \sum_{i=0}^{\infty} (a-b+1)_{2i} \frac{t^{2i}}{(2i)!} \left\{ 1 - \frac{[(a-b+1)+(2i)]}{(2i+1)} t \right\} \\ &= \sum_{i=0}^{n} (a-b+1)_{2i} \frac{t^{2i}}{(2i)!} \left\{ 1 - \frac{[(a-b+1)+(2i)]}{(2i+1)} t \right\} + \\ \mathrm{s}(a-b+1)_n & \sum_{i=n}^{\infty} \prod_{k=n}^{2i-1} [(a-b+1)+k] \frac{t^{2i}}{(2i)!} \left\{ 1 + \frac{(2i+1)-(a-b)}{(2i+1)} t \right\}. \end{aligned}$$

Inspection of the infinite sum reveals all positive terms. Consequently Fubini's theorem applies.

Transforming the integral creates a weighted sum of incomplete gamma functions:

$$\begin{aligned} M(a,b,-x) &= \frac{\Gamma(b) x^{-a}}{\Gamma(b-a)\Gamma(a)} \sum_{i=0}^{\infty} (a-b+1)_i \frac{1}{i! x^i} \int_0^x \exp(-u) u^{i+a-1} du \\ &= \frac{\Gamma(b) x^{-a}}{\Gamma(b-a)\Gamma(a)} \sum_{i=0}^{\infty} (a-b+1)_i \frac{1}{i! x^i} \gamma(x; i+a)\,. \end{aligned} \tag{4.4}$$

A second transformation leads to a weighted sum of Gamma random variable CDF's:

$$M(a,b,-x) = \frac{\Gamma(b)x^{-a}}{\Gamma(b-a)}\sum_{i=0}^{\infty}\frac{(a-b+1)_i(a)_i}{i!x^i}F_\gamma(x;i+a)\,. \tag{4.5}$$

The results also apply to $x > 0$ (with $b > a > 0$). Use the Kummer transformation to write

$$M(a,b,x) = \exp(x)\frac{\Gamma(b)x^{-(b-a)}}{\Gamma(a)\Gamma(b-a)}\sum_{i=0}^{\infty}\frac{(1-a)_i}{i!x^i}\gamma(x;i+b-a)\,, \tag{4.6}$$

or

$$M(a,b,x) = \exp(x)\frac{\Gamma(b)x^{a-b}}{\Gamma(a)}\sum_{i=0}^{\infty}\frac{(b-a)_i(1-a)_i}{i!x^i}F_\gamma(x;i+b-a)\,. \tag{4.7}$$

If $x \gg \nu$ then $F_\gamma(x;\nu) \approx 1$. The substitution reduces the new (exact) series representations in terms of $F_\gamma(x;\nu)$ into the asymptotic approximations described earlier. The relationship suggests when the asymptotic approximations will diverge before achieving the accuracy desired.

Method 4C; Continued Fraction for Exact Power Series in x^{-1} and Gamma's. For $x \gg 0$ write $A_{-1} = A_0 = 1$. For $M(a,b,x)$ let $A_1 = 1 + (b-a)(1-a)F_\gamma(x;b-a)/x$ and $r_i = [(b-a+i-1)(i-a)/i] \times [F_\gamma(x;i+b-a)/F_\gamma(x;i+b-a-1)]$ for $i > 1$. For $M(a,b,-x)$ let $A_1 = 1 + (1+a-b)aF_\gamma(x;a)/x$ and $r_i = [(a-b-i)(a-i-1)/i] \times [F_\gamma(x;i+a)/F_\gamma(x;i+a-1)]$. In either case: i) $A_i = A_{i-1} + (A_{i-1} - A_{i-2})r_i/x$, ii) $M_0 = 1$, and iii) for $i > 1$ compute the i^{th} approximant of the sum as $M_i = A_i$.

4.2 A New Series for $M(a,b,x)$ as the Expected Value of a Function of a Beta

Method 5; Power Series in x and Betas. A Beta random variable with parameters $\alpha > 0$ and $\delta > 0$ has $\mathcal{E}\beta(\alpha,\delta) = \alpha/(\alpha+\delta)$ and moment generating function $\phi(x) = M(\alpha,\alpha+\delta,x)$ (5, Chapter 25). Define $\mu_m = \mathcal{E}[\beta(\alpha,\delta) - \mathcal{E}\beta(\alpha,\delta)]^m$, with $\mu_0 = 1$ and $\mu_1 = 0$. For a positive integer m, write equation 25.16 in Johnson, *et al.* (5)

$$\mu_{m+1} = \frac{\alpha}{(\alpha+\delta)}\sum_{j=1}^{m}\binom{m}{j}\frac{(\alpha+\delta)^{-j}\left[1-\alpha(\alpha+\delta)^{-1}\right]^j j!}{\prod_{k=0}^{j}\left[1+(m-k)(\alpha+\delta)^{-1}\right]}\mu_{m-j} - \frac{\alpha m\mu_m}{(\alpha+\delta)(\alpha+\delta+m)} \tag{4.8}$$

$$= \alpha\sum_{j=1}^{m}\frac{\mu_{m-j}}{(\alpha+\delta+m-j)}\prod_{k=0}^{j-1}\frac{\delta(m-k)}{(\alpha+\delta)(\alpha+\delta+m-k)} - \frac{\alpha m\mu_m}{(\alpha+\delta)(\alpha+\delta+m)}\,.$$

Note that in Johnson, *et al.* the term $\alpha m\mu_m/[(\alpha+\delta)(\alpha+\delta+m)]$ lacks a required factor of $\alpha/(\alpha+\delta)$ (see the original, equation 8, p176, 13). Hence $\mu_2 = \alpha\delta/\left[(\alpha+\delta)^2(\alpha+\delta+1)\right]$ and $\mu_3 = 2\alpha\delta(\delta-\alpha)/\left[(\alpha+\delta)^3(\alpha+\delta+1)(\alpha+\delta+2)\right]$.

If $b > a > 0$ (for any x) then the integral form mentioned earlier allows writing $M(a,b,x)$ in terms of the moment generating function of $B = \beta(a,b-a)$:

$$M(a,b,x) = \frac{\Gamma(b)}{\Gamma(a)\Gamma(b-a)} \int_0^1 \exp(xt) t^{a-1} (1-t)^{b-a-1} dt \qquad (4.9)$$
$$= \mathcal{E}[\exp(xB)] .$$

Taking the expected value of a Taylor's series expansion of $\exp(xB)$ about $\mathcal{E}B = a/b$ implies

$$M(a,b,x) = \exp\Big(\frac{xa}{b}\Big) \sum_{m=0}^{\infty} \mu_m \frac{x^m}{m!} \qquad (4.10)$$
$$= \exp\Big(\frac{xa}{b}\Big) \left[1 + x^2 \sum_{i=0}^{\infty} \frac{\mu_{i+2}}{(i+2)!} x^i \right] .$$

The last form allows writing a continued fraction with $r_i = (\mu_{i+2}/\mu_{i+1})x/(i+2)$ for $i \geq 1$.

For B note that $\mu_2 = a(b-a)/[b^2(b+1)]$, $\mu_3 = 2a(b-a)(b-2a)/[b^3(b+1)(b+2)]$, and

$$\mu_{m+1} = a \sum_{j=1}^{m} \frac{\mu_{m-j}}{(b+m-j)} \prod_{k=0}^{j-1} \frac{(b-a)(m-k)}{b(b+m-k)} - \frac{am\mu_m}{b(b+m)} \qquad (4.11)$$
$$= a \sum_{j=0}^{m-1} \frac{\mu_j}{(b+j)} \prod_{k=j+1}^{m} \frac{(b-a)k}{b(b+k)} - \frac{am\mu_m}{b(b+m)} .$$

The terms in the infinite series have alternating sign if $b < 2a$ and $x > 0$, or if $b \geq 2a$ and $x < 0$. Other combinations yield all positive terms.

Method 5C; Continued Fraction for Power Series in x and Betas. Write $A_{-1} = A_0 = 1$ and $A_1 = 1$. For $i > 1$ compute $r_i = \mu_i/(i\mu_{i-1})$ and $A_i = A_{i-1} + (A_{i-1} - A_{i-2}) r_i x$. Then $M_0 = 1$, and for $i > 1$ compute the i^{th} approximant of the sum as $M_i = A_i$.

4.3 A Monte Carlo Method

The relationship to a Beta random variable for $b > a > 0$ allows using a simple simulation to approximate $M(a,b,x)$. First draw a random sample of realizations of $B = \beta(a, b-a)$. Second, compute $Y = \exp(xB)/\exp(xa/b) = \exp[x(B - a/b)]$ for each. Third, (carefully) tabulate the mean of Y. Finally, multiply the mean of Y by $\exp(xa/b)$. Large values of $R_1 = |xa/b|$ lead to computational difficulties.

5. NUMERICAL EVALUATIONS OF THE NEW METHODS

5.1 Methods and Design

A large number of enumerations of $M(a,b,x)$ helped evaluate the numerical accuracy of the three existing methods and the two new methods. Most of the same techniques as described in §3.1 were used here. The most important change was increasing the maximum number of terms to 300. In addition, a number of overflow checks were added to allow the modules to fail gracefully. Only the forwards algorithm was used for continued fractions. Each of the nine modules reported the value of the function, the number of terms evaluated, an error flag to indicate that divergence was detected by the module, and the vector of intermediate values. For Method 3 the module returned both numerator and denominator intermediate terms. In all cases both ln$[M(100,102,10)]$ and ln$[\exp(x)M(b-a,b,-x)]$ were tabulated separately. Hence a total of $9 \cdot 2 = 18$ function evaluations were computed for each choice of (a, b, x). A factorial design was used for each set of enumerations. Tables 1 and 2 contain lists of the values examined in the sets of enumerations reported in this paper.

Table 1
Sets of a and x, With $b = a + 2$, Tested for $M(a, b, x)$
All Combinations of a, b, and x Tested Within Each Set

Set	a	x
1.1	1, 10, 100	1, 10, 100
1.2	2.1, 8.1, 50.1, 100.1, 1000.1	10, 100, 1000, 2000, 4000, 8000
1.3	1	1000, 2000, 4000, 8000, 16000
1.4	1, 10, 100, 1000	8000
1.5	1, 10, 100	1, 10, 100
1.6	2.1, 8.1, 50.1, 100.1, 1000.1	10, 100, 1000

Table 2
Sets of j, n and x Tested for $M(n/2 + j, n/2 + 2j + 1, x)$
All Combinations of j, n, and x Tested Within Each Set

Set	j	n	x
2.1	0, 5	3, 100, 1000	10, 100, 1000, 2000, 8000, 16000
2.2	0, 5, 20	2000, 4000,8000, 16000	2000, 4000, 8000, 16000

Computational speed was examined for a small number of cases from sets 1.1-1.3 that required a large number of terms. This led to removing Methods 5 and 5C from sets 1.4-1.6 and 2.1-2.2. Subsequently a number of cases in those sets were computed with Methods 5 and 5C, but with the maximum number of terms reduced to 250, and then to 100.

Table 3
Performance of Nine Methods for Computing
$M(a, b, x) = \exp(x)M(b - a, b, -x)$,
With ln$[M(100, 102, 10)] = 9.8127$

		Method								
		1	2	3	4	5	1C	2C	4C	5C
x	# Terms	37	4	8	98	11	37	4	98	13
	log(max$\|$term$_i\|$)	3.4	3.6	-0.8	24.7	-2.0	3.4	2.5	24.7	0.0
	Error*		1		2			1	2	
$-x$	# Terms	12	4	8	98	11	12	4	98	13
	log(max$\|$term$_i\|$)	-0.7	3.6	-0.8	24.7	-2.0	-0.7	2.5	24.7	0.0
	Error*		1		2			1	2	

*Error = 1 if diverged, while error = 2 if diverged undetected by the module.

5.2 Results and Conclusions

Table 3 illustrates, for one combination of (a, b, x), the behavior of the various algorithms as they computed, or failed to compute, $M(a, b, x)$. Although not reported for the sake of brevity, the performance measures in Table 3 were tabulated and studied for all enumerations in this paper. In addition, the actual values reported by the algorithms were printed and studied. Values of $M(a, b, x)$ which did not approximately correspond to those predicted by simple interpolation from neighboring results allowed tracking down the serious error of divergence not detected by the module. Clear patterns arose from the many enumerations.

Table 4 contains all 17 "silent" failures that occurred, which involved a module incorrectly reporting convergence. Many less extreme values led to divergence detected by the modules. For example, with $a = 4000$, $b = 4001$, and $x = 4000$, only Method 3 converged. With $R_1 = |xa/b|$ and $R_2 = |a(b-a)/x|$, here $R_1 \approx 3999$, $R_2 \approx 1$. A few terms from Method 5 produces a good approximation, with the first one being $\exp(xa/b) = \exp(R_1)$.

Table 4
Silent Errors for Nine Methods of Computing
$M(a,b,x) = \exp(x)M(b-a,b,-x)$,
With $+$ If Error for $M(a,b,x)$ and $-$ If Error for $M(b-a,b,-x)$

					Method								
a	b	x	$R_1 \approx$	$R_2 \approx$	1	2	3	4	5	1C	2C	4C	5C
100.0	1.5	2.5	60.0	0.02	−					−			
6.5	12.5	100	52.0	0.39	−					−			
1.0	3.0	100	33.0	0.02	−					−			
2.1	4.1	100	51.0	0.04	−					−			
10.0	12.0	100	88.0	0.20	−				±	−			±
8.1	10.1	100	80.0	0.16	−				±	−			±
1.0	3.0	1	0.3	2.00		±					±		
1.0	3.0	10	3.0	0.20		±					±		
1020.0	1041.0	8000	7839.0	2.70			±						
1020.0	1041.0	16000	15677.0	1.30			±						
50.1	52.1	10	10.0	10.00				±				±	
100.1	102.1	10	10.0	20.00				±				±	
100.0	102.0	1	1.0	200.00				±				±	
100.0	102.0	10	10.0	20.00				±				±	
55.0	61.0	10	9.0	33.00				±				±	
505.0	511.0	10	10.0	303.00								±	
1.0	2.0	8000	4000.0	10^{-4}					±				

Conclusion 1. Except perhaps for some cases with Method 3, checks for overflow appear to always signal situations in which the module has failed.

Conclusion 2. The $i = 1$ term in the series predicts numerical performance of the methods. For Methods 1, 1C, 5, 5C, and, apparently 3, examine

$$R_1 = \left|x\frac{a}{b}\right|. \tag{5.1}$$

For Methods 2, 2C, 4 and 4C, if $x > 0$ examine $R_{2+} = |(1-a)(b-a)/x|$, while if $x < 0$ examine $R_{2-} = |a(1+a-b)/x|$. More loosely, define

$$R_2 = \left|\frac{a(b-a)}{x}\right|. \tag{5.2}$$

Except for the asymptotic series (Method 2), all series terms eventually vanish. Computational difficulty arises from intermediate terms with roughly the same number of significant digits as the precision of the software in use. For $i > 1$, the i^{th} terms behaves roughly like the first term to the i^{th} power. For example, if the software allows d digits of accuracy and $|xa/b|^i \approx 10^d$, then Methods 1 and 5 are likely to lose accuracy.

Conclusion 3. As many as 250 terms may be needed to achieve a relative precision of 10^{-10} for the implementations used here. However, a smaller limit would lose only a few valid results. Some failed computations will continue to the maximum number.

Conclusion 4. Using continued fractions occasionally extended the range of accuracy. More importantly, continued fractions rarely reduced accuracy, and then only slightly.

Conclusion 5. Method 1 seems accurate if $R_1 < 30$.

Conclusion 6. Method 2 seems accurate if $R_2 < 1$ and $x > 50$.

Conclusion 7. Method 3 works over the largest range of conditions, with $R_1 < 4000$. It continues to work accurately but increasingly slowly as R_1 increases.

Conclusion 8. Method 4, as a generalization of Method 2, extends the range of Method 2, at the cost of some computational speed.

Conclusion 9. Method 5 provides accuracy roughly like Method 1, except that a few terms from Method 5 provide an excellent approximation.

Conclusion 10. Method 5 may take roughly 100 times longer than any other, at least for large R_1. The speed difference increases exponentially in the number of terms required. The slowness arises from the need to completely recalculate each higher moment.

6. DISCUSSION

6.1 A General Strategy for Computing $M(a, b, x)$

With fixed precision, no single form allows computing $M(a, b, x)$ reliably to a specified accuracy for all inputs. The following steps provide a general strategy for real inputs. First, verify that the function is finite and well-defined. Finite (a, b, x) and b not zero or a negative integer suffices. Second, determine whether the calculation represents a special case, such as $a = b$, or a a negative integer. Use Kummer transformations and recurrence relations to reduce the calculation to a special case. For example, check if $b - a$ equals a negative integer. Third, failure to find a special case requires direct calculation.

The magnitudes of x, R_1 and R_2 should guide the choice of method. Use the Kummer transformation and compute R_1 and R_2 for both forms. Method 3 provides the best default choice. If $x > 50$ and $R_2 < 1$ then Method 4 will likely work well. Otherwise use Method 3 for the form with the smallest R_1. If both fail, then a few terms from Method 5 may work well.

6.2 Generalizations and Future Research

Computing $M(a, b, x)$ for extreme parameter values requires extreme care in implementing any algorithm as a computer program. Hence the focus here has been on accuracy first. Obviously computing speed and implementation efficiency merit attention. Note that in most cases at least two methods work well.

The results could be extended to complex variables in a straightforward way. Methods 1, 2 and 3 were all originally stated in terms of complex variables. The derivations for Methods 4 and 5 could be extended. Note that the software used here assumes real values.

REFERENCES

1. Abramowitz, M., and Stegun I. A., editors (1964) *Handbook of Mathematical Functions*, National Bureau of Standards Applied Mathematics Series, #55, Washington, D. C.: U. S. Printing Office.
2. Brent, R. P. (1980) Unrestricted algorithms for elementary and special functions, in S. H. Lavington (ed), *Information Processing 80*, 613-619, Amsterdam: North Holland Publishing.
3. Dingle, R. B. (1973) *Asymptotic Expansions: Their Derivation and Interpretation*, New York: Academic Press.
4. Jones, W. B. and Thron W. J. (1980) *Continued Fractions*, Reading, Mass.: Addison-Wesley.
5. Johnson, N. L., Kotz, S., and Balakrishnan, N. (1994) *Continuous Univariate Distributions-2*, New York: Wiley, 2nd ed.
6. Khatri, C. G., and Pillai K. C. S. (1967) On the moments of traces of two matrices in multivariate analysis, *Annals of the Institute of Statistical Mathematics*, **19**, 13-156.
7. Lauwerier, H. A. (1966) *Asymptotic Expansions*, Amsterdam: Mathematisch Centrum Amsterdam (Mathematical Centre Tracts #13).
8. Lebedev, N. N. (1965) *Special Functions and Their Applications* (translation by R. Silverman) Englewood Cliffs, New Jersey: Prentice Hall.
9. Luke, Y. L. (1977) *Algorithms for the Computation of Mathematical Functions*, New York: Academic Press.
10. Mathai, A. M. (1953) *A Handbook of Generalized Special Functions for the Statistical and Physical Sciences*, Oxford: Clarendon Press.
11. Morse, P. M. and Feshbach, H. (1953) *Methods of Theoretical Physics*, New York: McGraw Hill.

12. Muller, K. E., LaVange, L. M., Ramey, S. L., and Ramey, C. T. (1992) Power calculations for general linear multivariate models including repeated measures applications. *Journal of the American Statistical Association*, **87**, 1209-1226.

13. Mühlbach, G. (1972) Recursion formulae for the Pólya and Beta distributions, *Metrika*, **19**, 171-177. (in German)

14. Press, W. H., Teukolsky, S. A., Vetterling, W T., and Flannery B. P. (1992) *Numerical Recipes in Fortran*, New York: Cambridge University Press, 2nd ed.

15. Relph, A. P. (1963) Algorithm 192, confluent hypergeometric, *Communications of the Association of Computing Machinery*, **6**, 388.

16. SAS Institute Inc. (1989) *SAS/IML® Software: Usage and Reference, Version 6, First Edition*, Cary NC: SAS Institute Inc.

17. Slater, L. J. (1960) *Confluent Hypergeometric Functions*, Cambridge: Cambridge Press.

18. Temme, N. M. (1983) The numerical computation of the confluent hypergeometric function U(a,b,z), *Numerical Mathematics*, **41**, 63-82.

19. Thompson, W. J. (1997) *Atlas for Computing Mathematical Functions*, New York: Wiley.

20. van der Laan, C. G., and Temme N. M. (1984) *Calculation of Special Functions: the Gamma Function, the Exponential Integrals and Error-Like Functions*, Amsterdam: Centre for Mathematics and Computer Science.