An Algorithm For The Approximation Of Integrals With Exact Error Bounds

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Abstract

An iterative algorithm is developed for constructing upper and lower bounds for the value of an integral. The methodology can be used to obtain approximations of exact absolute or relative accuracy. Based on the concavity structure of a derivative of the integrand, the algorithm is relatively simple to implement and is highly efficient when the order of the derivative is modest. While the theory is developed for integrals of arbitrary dimension the methodology will be useful primarily for lower dimensional integrals. This is demonstrated through applications to the evaluation of distribution functions and special functions of interest in probability and statistics. Also bounds on tail probabilities are developed that can be considered to be a generalization of the Mills' ratio inequality for the standard normal.

1 Introduction

Suppose that we want to construct an approximation to an integral $\int_a^b f(x)\,dx$ with some prescribed accuracy ϵ; i.e. the value reported is guaranteed to be within ϵ of the true value with respect to either absolute or relative error. The need to calculate accurate approximations to such one dimensional integrals arises quite commonly in probability and statistics via distribution functions, expectations, etc. As a practical issue one would like to have available relatively general methods that permit the construction of efficient algorithms for such approximations. Standard references such as Kennedy

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and Gentle (1980), Davis and Rabinowitz (1984), Thisted (1988) and Press, Flannery, Teukolsky and Vetterling (1986) discuss methods for approximating such integrals.

The approach that we present has some virtues from the point of view of its simplicity, efficiency and the fact that, with some qualifications due to round-off error, it returns exact error bounds along with the approximate value. Often the methodology leads to good algorithms with relatively little work from the implementer. For example, evaluation of the $N(0, 1)$ distribution function is a much studied problem and when we consider the application of our methodology to this problem in Example 4.2 we obtain surprisingly good results with very little effort. Similarly we obtain good results in Example 4.3 where we apply the methodology to constructing approximations to the Gamma function and the Gamma distribution function. In Example 4.4 we show that the technique can be used to evaluate an approximation to a non-standard problem having application in actuarial science; namely Makeham's distribution function.While we have emphasized the application of the methodology to one dimensional integrals the method can be generalized to multidimensional integrals. We illustrate this in in Example 4.5 where we compute approximations to the probability contents of rectangles for the bivariate Student distribution.

In Gilks and Wild (1992), Hoermann (1995) and Evans and Swartz (1996) a class of techniques with common characteristics is discussed for constructing random variable generators from a univariate density. The basic idea behind these methods involves piecewise linear approximations to a transformation of the density to construct upper and lower envelopes for the density. The virtue of this methodology is that it requires very little input from the user beyond the choice of a transformation and knowledge of the concavity structure of the transformed density or equivalently the inflection points of the transformed density. It is to a great degree a black-box generator.

The upper and lower envelopes constructed via these algorithms also lead to easily calculated upper and lower approximations to the associated distribution function and so we can compute approximations with exact error bounds. Such integration techniques might be referred to as *envelope rules*. The approximation to the integral obtained from the lower envelope is in fact an application of the trapezoid rule with an additional restriction on the placement of the integration points. As we show in this paper, however, while this methodology is excellent for constructing random variable generators it can be very inefficient for approximating distribution functions. In section 2 we show that this is due to the low order of the rate of convergence of the methodology as an integration technique. We also show, however, that this methodology can be generalized to yield integration techniques of any rate of convergence provided that information concerning the concavity structure of the derivatives of the density is available. This information is either available or, as we show, is even unneccessary, for many commonly used distributions. In section 3 we generalize the algorithm to multidimensional contexts. In section 4 we apply the methodology to a number of examples.

In developing upper and lower bounds for integrals in this paper we ignore the effects of round-off error. In practice this means that actual bounds computed may not contain the true value of the integral. True bounds can be attained, however, if we combine the methods of interval arithmetic with our algorithms. We do not pursue this aspect of the computation here. For a discussion of the use of interval arithmetic in the approximation of distribution functions see Wang and Kennedy (1994).

The methods we derive here involve the use of Taylor expansions of the integrand and their direct integration. Lyness (1969) also uses Taylor expansions in the approximation of integrals but the development there is quite different from what we are proposing.

2 The Algorithm for One Dimensional Integrals

We assume hereafter that an integrand f possesses the number of derivatives necessary to make the results stated below valid. The basic idea behind the algorithm is dependent on the following simple fact derived from the Fundamental Theorem of Calculus.

Lemma 1. If $f^{'}(x) \leq g^{'}(x)$ for every $x \in (a,b)$ then $f(x) \leq g(x) - g(a) + f(a)$ for every $x \in (a,b)$.

Now suppose that f is a density function such that $f^{(n)}$ is concave in (a,b). Then we have the following result which gives upper and lower envelopes for f on (a,b).

Lemma 2. If $f^{(n)}$ is concave on (a,b) then for every $x \in (a,b)$,

$$\begin{aligned} l(x) &= \sum_{k=0}^{n} \frac{f^{(k)}(a)}{k!}(x-a)^k + \frac{f^{(n)}(b) - f^{(n)}(a)}{b-a} \frac{(x-a)^{n+1}}{(n+1)!} \\ &\leq f(x) \leq u(x) = \sum_{k=0}^{n+1} \frac{f^{(k)}(a)}{k!}(x-a)^k. \end{aligned} \quad (1)$$

Proof. Because $f^{(n)}$ is concave on (a, b) we have that the chord

$$l^{(n)}(x) = f^{(n)}(a) + \frac{f^{(n)}(b) - f^{(n)}(a)}{b-a}(x-a)$$

and the tangent

$$u^{(n)}(x) = f^{(n)}(a) + f^{(n+1)}(a)(x-a)$$

satisfy $l^{(n)}(x) \leq f^{(n)}(x) \leq u^{(n)}(x)$ on (a, b). Then repeatedly applying Lemma 1 to both sides of this inequality we obtain the result.

Corollary 1. Integrating both sides of (1) gives

$$\begin{aligned} & \sum_{k=0}^{n} \frac{f^{(k)}(a)}{(k+1)!}(b-a)^{k+1} + \frac{f^{(n)}(b) - f^{(n)}(a)}{b-a} \frac{(b-a)^{n+2}}{(n+2)!} \\ \leq \quad & \int_a^b f(x)\,dx \leq \sum_{k=0}^{n+1} \frac{f^{(k)}(a)}{(k+1)!}(b-a)^{k+1}. \end{aligned} \tag{2}$$

Accordingly, (2) gives upper and lower bounds for $\int_a^b f(x)\,dx$ and this implies that an upper bound on the absolute error in the approximation $\int_a^b u(x)\,dx$ to $\int_a^b f(x)\,dx$ is given by

$$\left(f^{(n+1)}(a) - \frac{f^{(n)}(b) - f^{(n)}(a)}{b-a} \right) \frac{(b-a)^{n+2}}{(n+2)!}. \tag{3}$$

If $f^{(n)}$ is convex on (a, b) then the inequalities in (1) and (2) are reversed and (3) is multiplied by -1. The bound (3) can be used to give insight concerning the choice of n.

Notice that $\int_a^b u(x)\,dx = \int_a^b f(x)\,dx$ whenever f is a polynomial of degree less than $n+2$ and $\int_a^b l(x)\,dx = \int_a^b f(x)\,dx$ whenever f is a polynomial of degree less than $n+1$. While we have stated the results for concave or convex $f^{(n)}$ the technique is also applicable when these conditions do not apply. For, provided that we can determine the inflection points of $f^{(n)}$ in (a, b), namely the roots of $f^{(n+2)}$, we can then determine the concavity of $f^{(n)}$ on each of the subintervals determined by these points and apply the results piecewise. Recall that the concavity on each of these intervals is determined by the sign of $f^{(n+3)}$ at the inflection points.

If (a, b) is short then we can imagine that the approximations $\int_a^b u(x)\,dx$ and $\int_a^b l(x)\,dx$ will be quite good. In the typical application, however, this will not be the case. We now show, however, that under componding these approximations converge to the value of the integral. By compounding we mean divide (a, b) into m subintervals of equal length, use the approximations to the integral over this subinterval given by Corollary 1, and then sum the approximations. Let l_m, u_m denote the lower and upper envelopes to f on (a, b) determined by this compounding; i.e. the envelopes determined by applying Lemma 1 in each subinterval. The following result establishes the convergence of the approximations $\int_a^b u_m(x)\,dx$ and $\int_a^b l_m(x)\,dx$ and the rate of convergence as $m \to \infty$.

Lemma 3. If $E^m$and E_m denote the errors in $\int_a^b u_m^{(n)}(x)\,dx$ and $\int_a^b l_m^{(n)}(x)\,dx$ respectively then as $m \to \infty$ we have

$$\begin{aligned}
E^m &\sim \frac{1}{m^{n+2}}\left(f^{(n+1)}(b) - f^{(n+1)}(a)\right)\frac{(b-a)^{n+2}}{(n+3)!} \to 0 \\
E_m &\sim (n+3)\,\frac{1}{m^{n+2}}\left(f^{(n+1)}(b) - f^{(n+1)}(a)\right)\frac{(b-a)^{n+2}}{(n+3)!} \to 0.
\end{aligned}$$

Proof. ¿From Taylor's Theorem we have that

$$f(x) = u(x) + f^{(n+2)}(\zeta(x))\frac{(x-a)^{n+2}}{(n+2)!}$$

where $\zeta(x) \in (a, b)$. Therefore

$$\begin{aligned}
\int_a^b f(x)\,dx &= \int_a^b u(x)\,dx + \int_a^b f^{(n+2)}(\zeta(x))\frac{(x-a)^{n+2}}{(n+2)!}\,dx \\
&= \int_a^b u(x)\,dx + f^{(n+2)}(\tau)\int_a^b \frac{(x-a)^{n+2}}{(n+2)!}\,dx \\
&= \int_a^b u(x)\,dx + f^{(n+2)}(\tau)\frac{(b-a)^{n+3}}{(n+3)!}
\end{aligned}$$

where the second equality is justified by the Generalized Mean Value Theorem, see Davis and Rabinowitz (1984, p. 9). Also by Taylor's Theorem

$$f(x) = l(x) + \left[f^{(n+1)}(\eta(x)) - \frac{f^{(n)}(b) - f^{(n)}(a)}{b-a}\right]\frac{(x-a)^{n+1}}{(n+1)!}$$

where $\eta(x) \in (a, b)$, which gives

$$\int_a^b f(x)\,dx$$

$$
\begin{aligned}
&= \int_a^b l(x)\,dx + \int_a^b \left[f^{(n+1)}(\eta(x)) - \frac{f^{(n)}(b) - f^{(n)}(a)}{b-a} \right] \frac{(x-a)^{n+1}}{(n+1)!}\,dx \\
&= \int_a^b l(x)\,dx + \left[f^{(n+1)}(\xi) - \frac{f^{(n)}(b) - f^{(n)}(a)}{b-a} \right] \int_a^b \frac{(x-a)^{n+1}}{(n+1)!}\,dx \\
&= \int_a^b l(x)\,dx + \left[f^{(n+1)}(\xi) - f^{(n+1)}(\xi^*) \right] \frac{(b-a)^{n+2}}{(n+2)!} \\
&= \int_a^b l(x)\,dx + f^{(n+2)}(\xi^{**}) \frac{(b-a)^{n+3}}{(n+2)!}
\end{aligned}
$$

where the second equality is justified by the Generalized Mean Value Theorem for some $\xi \in (a,b)$ and the last two equalities are justified by the usual Mean Value Theorem for some $\xi^*, \xi^{**} \in (a,b)$. The statements in the Lemma then follow immediately from the theorem on p. 72, Davis and Rabinowitz (1984).

Therefore both approximations have the same rate of convergence under compounding but E_m has a larger constant. For this reason we use the integral of the upper envelope as the basic approximation. Note that when $n = 0$ then the rate of convergence is quadratic; i.e $O(1/m^2)$. As we shall see in section 4, this proves inadequate in a number of examples as it requires far too much compounding. Dramatic improvements are obtained by using higher order derivatives.

The integration algorithm that we have presented can be generalized in several ways. For example, suppose that $f(x) = g(x)h(x)$, $g(x) \geq 0, l(x) \leq h(x) \leq u(x)$ on (a,b) where l and u are as specified in (1) for h rather than f. Then $g(x)l(x) \leq f(x) \leq g(x)u(x)$ holds on (a,b). Also assume that that g and h have all the necessary derivatives and that all necessary integrals exist. Then, with a proof similar to that of Lemma 3, we have the following result.

Lemma 4. If $E^m$and E_m denote the errors in $\int_a^b g(x)u_m(x)\,dx$ and $\int_a^b g(x)l_m(x)\,dx$ respectively then as $m \to \infty$

$$
\begin{aligned}
E^m &\sim \frac{1}{m^{n+2}} \left(\int_a^b g(x)h^{(n+2)}(x)\,dx \right) \frac{(b-a)^{n+2}}{(n+3)!} \to 0 \\
E_m &\sim (n+3)\,\frac{1}{m^{n+2}} \left(\int_a^b g(x)h^{(n+2)}(x)\,dx \right) \frac{(b-a)^{n+2}}{(n+3)!} \to 0.
\end{aligned}
$$

If g represents a great deal of the variability in f then we might expect these approximations to improve on applying the theory strictly to f. Of course

g must also be chosen so that $\int_a^b g(x)u_m(x)\,dx$ and $\int_a^b g(x)l_m(x)\,dx$ can be easily evaluated; see Example 4.3 for such an application.

Sometimes we can write $f(x) = h(g(x))$. Let l and u be as specified in (1) but for h on (c, d) and suppose $g(x) \in (c, d)$ whenever $x \in (a, b)$. Then $l(g(x)) \le f(x) \le u(g(x))$ holds on (a, b). Assuming that g and h have all the necessary derivatives and that all necessary integrals exist then, with a proof similar to that of Lemma 3, we have the following result.

Lemma 5. If E^m and E_m denote the errors in $\int_a^b u_m(g(x))\,dx$ and $\int_a^b l_m(g(x))\,dx$ respectively then as $m \to \infty$

$$\begin{aligned} E^m &\sim \frac{1}{m^{n+2}}\left(\int_a^b h^{(n+2)}(g(x))\,dx\right)\frac{(b-a)^{n+2}}{(n+3)!} \to 0 \\ E_m &\sim (n+3)\frac{1}{m^{n+2}}\left(\int_a^b h^{(n+2)}(g(x))\,dx\right)\frac{(b-a)^{n+2}}{(n+3)!} \to 0. \end{aligned}$$

Again g must be chosen so that $\int_a^b u_m(g(x))\,dx$ and $\int_a^b l_m(g(x))\,dx$ can be easily evaluated; see Example 4.2 for such an application. Lemmas 4 and 5 can be used to substantially simplify and improve the application of the method.

We will make use of the following simple facts when calculating absolute and relative error bounds in our examples. Suppose that we wish to approximate quantities r and s and that we have lower bounds l_r, l_s and upper bounds u_r, u_s. Then we have that $l_r + l_s \le r + s \le u_r + u_s$ and therefore $(u_r + u_s) - (l_r + l_s)$ is an absolute error bound for the approximations $u_r + u_s$ and $l_r + l_s$ of $r + s$. Further if l_s is positive then $l_r/u_s \le r/s \le u_r/l_s$ and $u_r/l_s - l_r/u_s$ is an absolute error bound for the approximations u_r/u_s and l_r/l_s of r/s. Further, when l_r is positive then the absolute relative error in u_r as an approximation of r is bounded above by $u_r/l_r - 1$. Similarly, we can combine lower and upper bounds on quantities to compute bounds on the absolute and absolute relative errors of other simple functions of those quantities.

3 The Algorithm for Multidimensional Integrals

We can also generalize the methodology to multivariate contexts. Once again we will assume that all the necessary derivatives exist for the validty of any stated results. For integrand $f : R^p \to R$ we say that the *n-th* derivative $d^n f$ is concave in open, convex $C \subseteq R^p$ if the *n-th* order directional derivative

$d^n f_\alpha(\beta,\ldots,\beta)$ is a concave function of $\alpha \in C$ for every $\beta \in R^p$ and recall that

$$d^n f_\alpha(\beta,\ldots,\beta) = \sum_{j_1+\cdots+j_p=n} \left(\begin{array}{c} n \\ j_1 \cdots j_p \end{array} \right) \frac{\partial^n f(\alpha)}{\partial \alpha_1^{j_1} \cdots \partial \alpha_p^{j_p}} \beta_1^{j_1} \cdots \beta_p^{j_p}. \quad (4)$$

This implies that $d^n f_{\alpha+t\beta}(\beta,\ldots,\beta)$ is a concave function of t provided $\alpha + t\beta \in C$. Then as in section 2, for $0 \le t \le 1$ we have

$$\begin{aligned} & d^n f_\alpha(\beta,\ldots,\beta) + t\left(d^n f_{\alpha+\beta}(\beta,\ldots,\beta) - d^n f_\alpha(\beta,\ldots,\beta)\right) \\ \le\ & d^n f_{\alpha+t\beta}(\beta,\ldots,\beta) \\ \le\ & d^n f_\alpha(\beta,\ldots,\beta) + t d^{n+1} f_\alpha(\beta,\ldots,\beta) \end{aligned} \quad (5)$$

provided that $\alpha, \alpha+\beta \in C$. Then using t as the variable of integration in the right-hand side of (5), anti-differentiating n times as in section 2, and putting $t = 1, \beta = z - \alpha$ we obtain an upper envelope for f given by

$$u(z) = \sum_{k=0}^{n+1} \frac{d^k f_\alpha(z-\alpha,\ldots,z-\alpha)}{k!}$$

when $\alpha, z \in C$. Therefore we need only integrate polynomials over C to get an upper bound on $\int_C f(z)\,dz$. For the lower bound we assume in addition that C is relatively compact, antidifferentiate the left-hand side of (5) n times and put $t = 1, \beta = z - \alpha$ to obtain

$$\begin{aligned} f(z) \ \ge\ & \sum_{k=0}^{n} \frac{d^k f_\alpha(z-\alpha,\ldots,z-\alpha)}{k!} + \\ & \frac{\left(d^n f_z(z-\alpha,\ldots,z-\alpha) - d^n f_\alpha(z-\alpha,\ldots,z-\alpha)\right)}{(n+1)!} \end{aligned}$$

This lower bound is typically not useful here, however, because of the $d^n f_z$ term as this cannot be easily integrated.

In the most important context, however, a useful lower bound can be computed. For this consider the rectangle $[a,b] = \prod_{i=1}^p [a_i, b_i] \subseteq C$ and let $\alpha = a$ and note that when $z \in [a,b]$ each coordinate of $\beta = z - \alpha$ is non-negative. Denote the set of vertices of the rectangle $[a,b]$ by $[a,b]^*$. Now from the concavity we have that $d^n f_w(\beta,\ldots,\beta)$ is minimized for $w \in [a,b]$ at a value $w \in [a,b]^*$. Therefore for $w \in [a,b]$ and $\beta = z - \alpha$ with $z \in [a,b]$,

$$\begin{aligned} & d^n f_w(\beta,\ldots,\beta) - d^n f_\alpha(\beta,\ldots,\beta) \\ \ge\ & \min_{w^* \in [a,b]^*} \left\{ d^n f_{w^*}(\beta,\ldots,\beta) - d^n f_\alpha(\beta,\ldots,\beta) \right\} \end{aligned}$$

$$\geq \min_{\substack{w^* \in [a,b]^* \\ j_1+\cdots+j_p=n}} \left\{ \frac{\partial^n f(w^*)}{\partial\alpha_1^{j_1}\cdots\partial\alpha_p^{j_p}} - \frac{\partial^n f(\alpha)}{\partial\alpha_1^{j_1}\cdots\partial\alpha_p^{j_p}} \right\} (\beta_1+\cdots+\beta p)^n$$

$$= c^n(f,a,b)(\beta_1+\cdots+\beta p)^n .$$

This leads to the inequality $d^n f_\alpha(\beta,\ldots,\beta) + tc^n(f,a,b)(\beta_1+\cdots+\beta p)^n \leq d^n f_{\alpha+t\beta}(\beta,\ldots,\beta)$ and note that $c^n(f,a,b)$ can be computed relatively easily provided p and n are not large. Antidifferentiating this inequality n times in t and then putting $t=1, \alpha=a$ and $\beta=z-\alpha$ gives the lower envelope

$$l(z) = \sum_{k=0}^{n} \frac{d^k f_\alpha(z-\alpha,\ldots,z-\alpha)}{k!} + \frac{c^n(f,a,b)}{(n+1)!}(z_1-\alpha_1+\cdots+z_p-\alpha_p)^n .$$

The function l can be easily exactly integrated over $[a,b]$ to give a lower bound on $\int_{[a,b]} f(z)\,dz$. Note that $l(z)$ here is not a generalization of the one dimensional definition.

Consider now the approximations $\int_{[a,b]} l_{m^p}(z)\,dz$ and $\int_{[a,b]} u_{m^p}(z)\,dz$ where l_{m^p} and u_{m^p} are the lower and upper envelopes to f on $[a,b]$ obtained by compounding this approach. By compounding we now mean to subdivide $[a,b]$ into m^p subrectangles of equal volume by subdividing each edge of $[a,b]$ into m subintervals of equal length. We have the following result.

Lemma 7. If E_{m^p} and E^{m^p} denote the errors in the approximations $\int_{[a,b]} l_{m^p}(z)\,dz$ and $\int_{[a,b]} u_{m^p}(z)\,dz$ then as $m\to\infty$

$$E^{m^p} \sim \frac{1}{m^{n+2}} \sum_{j_1+\cdots+j_p=n+2} \begin{pmatrix} n+2 \\ j_1\ldots j_p \end{pmatrix} \int_{[a,b]} \frac{\partial^{n+2} f(z)}{\partial\alpha_1^{j_1}\cdots\partial\alpha_p^{j_p}}\,dz \times \frac{(b_1-a_1)^{j_1}\cdots(b_p-a_p)^{j_p}}{(j_1+1)\cdots(j_p+1)(n+2)!} \to 0$$

and $E_{m^p} = O(\frac{1}{m^{n+1}}) \to 0$.

Proof: As in Lemma 3 we use Taylor's Theorem, the Generalized Mean Value Theorem and (4) to establish

$$\int_{[a,b]} f(z)\,dz$$

$$= \int_{[a,b]} u(z)\,dz + \int_{[a,b]} \frac{d^{n+2} f_{\zeta(z)}(z-a,\ldots,z-a)}{(n+2)!}dz$$

$$= \int_{[a,b]} u(z)\,dz + \sum_{j_1+\cdots+j_p=n+2} \begin{pmatrix} n+2 \\ j_1\ldots j_p \end{pmatrix} \frac{\partial^{n+2} f(\tau(j_1,\ldots,j_p))}{\partial\alpha_1^{j_1}\cdots\partial\alpha_p^{j_p}}$$

$$
\begin{aligned}
& \times \int_{[a,b]} \frac{(z_1-a_1)^{j_1}\cdots(z_p-a_p)^{j_p}}{(n+2)!} dz \\
= \quad & \int_{[a,b]} u(z)\,dz + \sum_{j_1+\cdots+j_p=n+2} \left(\begin{array}{c} n+2 \\ j_1 \ldots j_p \end{array} \right) \frac{\partial^{n+2} f\left(\tau\left(j_1,\ldots,j_p\right)\right)}{\partial\alpha_1^{j_1}\cdots\partial\alpha_p^{j_p}} \\
& \times \frac{(b_1-a_1)^{j_1+1}\cdots(b_p-a_p)^{j_p+1}}{(j_1+1)\cdots(j_p+1)\,(n+2)!} \\
= \quad & \int_{[a,b]} u(z)\,dz + \sum_{j_1+\cdots+j_p=n+2} \left(\begin{array}{c} n+2 \\ j_1 \ldots j_p \end{array} \right) \frac{\partial^{n+2} f\left(\tau\left(j_1,\ldots,j_p\right)\right)}{\partial\alpha_1^{j_1}\cdots\partial\alpha_p^{j_p}} Vol([a,b]) \\
& \times \frac{(b_1-a_1)^{j_1}\cdots(b_p-a_p)^{j_p}}{(j_1+1)\cdots(j_p+1)\,(n+2)!}
\end{aligned}
$$

where $\zeta(z), \tau\left(j_1,\ldots,j_p\right) \in [a,b]$. This leads immediately to the expression for E^{m^p} via the same argument for the proof of the theorem on p. 72 of Davis and Rabinowitz (1984).

Similarly we have

$$
\begin{aligned}
& \int_{[a,b]} f(z)\,dz \\
= \quad & \int_{[a,b]} l(z)\,dz + \int_{[a,b]} \frac{d^{n+1} f_{\zeta(z)}\ (z-a,\ldots,z-a)}{(n+1)!} dz \\
& - \frac{c^n(f,a,b)}{(n+1)!} \int_{[a,b]} (z_1-a_1+\cdots+z_p-a_p)^n\ dz \\
= \quad & \int_{[a,b]} l(z)\,dz + \sum_{j_1+\cdots+j_p=n+1} \left(\begin{array}{c} n+1 \\ j_1 \ldots j_p \end{array} \right) \frac{\partial^{n+1} f\left(\tau\left(j_1,\ldots,j_{n+1}\right)\right)}{\partial\alpha_1^{j_1}\cdots\partial\alpha_p^{j_p}} Vol([a,b]) \\
& \times \frac{(b_1-a_1)^{j_1}\cdots(b_p-a_p)^{j_p}}{(j_1+1)\cdots(j_p+1)\,(n+1)!} \\
& - \left[c^n(f,a,b) Vol([a,b])\right] \frac{1}{(n+1)!} \sum_{k_1+\cdots+k_p=n} \left(\begin{array}{c} n \\ k_1 \ldots k_p \end{array} \right) \\
& \times \frac{(b_1-a_1)^{k_1}\cdots(b_p-a_p)^{k_p}}{(k_1+1)\cdots(k_p+1)}.
\end{aligned}
$$

Now observe that for $w^* \in [a,b]^*$ the Mean Value Theorem implies

$$
\frac{\partial^n f\left(w^*\right)}{\partial\alpha_1^{j_1}\cdots\partial\alpha_p^{j_p}} - \frac{\partial^n f\left(a\right)}{\partial\alpha_1^{j_1}\cdots\partial\alpha_p^{j_p}} = \sum_{i=1}^{p} \left(w_i^* - a_i\right) \frac{\partial^{n+1} f\left(\tau\left(j_1,\ldots,j_p\right)\right)}{\partial\alpha_1^{j_1}\cdots\partial\alpha_i^{j_i+1}\cdots\partial\alpha_p^{j_p}}
$$

for some $\tau\left(j_1,\ldots,j_p\right)$ on the line between a and w^* and thus $\tau\left(j_1,\ldots,j_p\right) \in [a,b]$, and note that $w_i^* - a_i = 0$ or $w_i^* - a_i = b_i - a_i$. From this we deduce that

$$|c^n(f,a,b)| \leq \sum_{i=1}^{p} (b_i - a_i) \max_{\substack{w \in [a,b] \\ j_1 + \cdots + j_p = n+1}} \left| \frac{\partial^{n+1} f(w)}{\partial \alpha_1^{j_1} \cdots \partial \alpha_p^{j_p}} \right|.$$

Therefore for all m large enough $|E_{m^p}| \leq \frac{K}{m^{n+1}}$ whenever K satisfies

$$\begin{aligned} K \quad > \quad & \sum_{j_1+\cdots+j_p=n+1} \left(\begin{array}{c} n+1 \\ j_1 \ldots j_p \end{array} \right) \int_{[a,b]} \left| \frac{\partial^{n+1} f(z)}{\partial \alpha_1^{j_1} \cdots \partial \alpha_p^{j_p}} \right| dz \times \\ & \frac{(b_1-a_1)^{j_1} \cdots (b_p-a_p)^{j_p}}{(j_1+1)\cdots(j_p+1)(n+1)!} \\ & + \left(\sum_{i=1}^{p} (b_i - a_i) \right) \max_{\substack{w \in [a,b] \\ j_1 + \cdots + j_p = n+1}} \left| \frac{\partial^{n+1} f(w)}{\partial \alpha_1^{j_1} \cdots \partial \alpha_p^{j_p}} \right| \times \\ & \sum_{k_1+\cdots+k_p=n} \left(\begin{array}{c} n \\ k_1 \ldots k_p \end{array} \right) \frac{(b_1-a_1)^{k_1+1} \cdots (b_p-a_p)^{k_p+1}}{(k_1+1)\cdots(k_p+1)(n+1)!}. \end{aligned}$$

Observe that the result for the lower bound in Lemma 7 is not strictly a generalization of Lemma 3. We do better with one dimensional integrals to use the lower envelope approximation of section 2. It is possible that a better lower envelope approximation can be found in the multivariate context. Also observe that if we put $N = m^p$ then the rate of convergence of the upper approximation is $N^{-(\frac{n+2}{p})}$ and for the lower approximation $N^{-(\frac{n+1}{p})}$. So we need to choose n higher as we increase dimension if we want to achieve good results. The downside of this of course is the need to compute many derivatives. The above also assumes that regions of concavity of $d^n f_\alpha(\beta, \ldots, \beta)$ can be easily determined and this is not necessarily the case.

All of this suggests that the multivariate generalization is not very useful. Fortunately, we can obtain generalizations of Lemma 7 similar to the generalizations we obtained for Lemma 3 and these increase the utility of the methodolgy substantially. We illustrate this in Example 4.

4 Examples

4.1 The Exponential Distribution

Of course it is easy to calculate $F(x) = \int_0^x e^{-z}\,dz = 1 - e^{-x}$ but as we see in subsequent examples, the upper and lower envelopes to the function e^{-z} are very useful. Note that $(e^{-z})^{(n)} = (-1)^{(n)}\,e^{-z}$ and so the $n-th$ derivative is concave when n is odd and convex when n is even. Therefore on the interval (a,b), using the $n-th$ derivative, we obtain the upper envelope for e^{-z} given by

$$u^{(a,b)}(z) = \begin{cases} e^{-a}\sum_{k=0}^{n+1}\frac{(-1)^k}{k!}(x-a)^k & n\ odd \\ e^{-a}\sum_{k=0}^{n}\frac{(-1)^k}{k!}(x-a)^k + \frac{(-1)^n}{(n+1)!}\frac{e^{-b}-e^{-a}}{b-a}(x-a)^{n+1} & n\ even \end{cases}$$

and the lower envelope for e^{-z} given by

$$l^{(a,b)}(z) = \begin{cases} e^{-a}\sum_{k=0}^{n}\frac{(-1)^k}{k!}(x-a)^k + \frac{(-1)^n}{(n+1)!}\frac{e^{-b}-e^{-a}}{b-a}(x-a)^{n+1} & n\ odd \\ e^{-a}\sum_{k=0}^{n+1}\frac{(-1)^k}{k!}(x-a)^k & n\ even. \end{cases}$$

This implies that the absolute error in the approximation $\int_a^b u^{(a,b)}(z)\,dz$ to $\int_a^b e^{-z}\,dz$ is bounded above by $e(a,b,n) = \frac{(b-a)^{n+2}}{(n+2)!}\left(\frac{e^{-b}-e^{-a}}{b-a} + e^{-a}\right)$. For example, $e(0,1,5) = 7.3\times 10^{-5}, e(0,1,21) = 1.42\times 10^{-23}$ and $e(9,10,5) = 9.01\times 10^{-9}, e(9,10,21) = 1.76\times 10^{-27}$. The encouraging information from this is the potential for highly accurate approximations in other problems with very little computational effort.

4.2 The Normal Distribution Function

Many authors have discussed the approximation of the $N(0,1)$ distribution function $F(x) = \int_{-\infty}^x f(z)\,dz$ where $f(z) = \frac{1}{\sqrt{2\pi}}\exp\left(-\frac{1}{2}z^2\right)$. We consider applying our methods to this problem to assess performance in a well-known context. As it turns out there are several possibilities.

A strict application of our methodology involves computing

$$f^{(n)}(z) = (-1)^n\,H_n(z)f(z)$$

where H_n is the $n-th$ degree Hermite polynomial associated with f. These polynomials are obtained via the recursion $H_{n+1}(z) = zH_n(z) - nH_{n-1}(z)$ and $H_0(z) = 1, H_1(z) = z$. The concavity structure of $f^{(n)}$ is then obtained by calculating the roots of $H_{n+2}(z)$, as these give the inflection points of $f^{(n)}$, and observing the sign of $f^{(n+3)}$ at each of these points. Note that these inflection points are precisely the Gauss points of Gaussian integration rules. These values are readily available from common numerical packages.

Another approach to this problem is based on the observations that $F(-x) = 1 - F(x)$ and $F(0) = \frac{1}{2}$. Therefore we only need to consider $x > 0$ and compute $\int_0^x f(z)\,dz$. The upper and lower envelopes for f on $(c, d) \subseteq (0, x)$ are immediately available via $\frac{1}{\sqrt{2\pi}} u^{(a,b)}\left(\frac{z^2}{2}\right)$ and $\frac{1}{\sqrt{2\pi}} l^{(a,b)}\left(\frac{z^2}{2}\right)$ where $u^{(a,b)}$ and $l^{(a,b)}$ are as in Example 4.1 and $a = \frac{c^2}{2}$, $b = \frac{d^2}{2}$. These envelopes can be easily integrated exactly over (c, d) via the recursion

$$\begin{aligned}\int_c^d (z-c)^p (z+c)^q \, dz &= \frac{(d-c)^p (d+c)^{q+1}}{q+1} \\ &\quad - \frac{p}{q+1} \int_c^d (z-c)^{p-1} (z+c)^{q+1} \, dz\end{aligned}$$

for $p, q \in N$ and noting that $\left(z^2 - c^2\right)^k = (z-c)^k (z+c)^k$.

Neither of these methods will work well if x is too large. We note, however, that f is log-concave and the tangent to $\ln(f)$ at x is given by $\ln\left(\frac{1}{\sqrt{2\pi}} e^{-\frac{1}{2}x^2}\right) - x(z-x)$ and this has a negative slope when $x > 0$. Therefore

$$\begin{aligned}\int_x^\infty f(z)\,dz &\leq \int_x^\infty \exp\left(\ln\left(\frac{1}{\sqrt{2\pi}} e^{-\frac{1}{2}x^2}\right) - x(z-x)\right) dz \\ &= \frac{1}{\sqrt{2\pi}} \frac{e^{-\frac{1}{2}x^2}}{x} = \eta_x.\end{aligned}$$

If we wish to compute an approximation with absolute error less than ϵ and if $\eta_x < \epsilon$ then we return the the interval $(1 - \eta_x, 1)$ for the correct value. If our criterion is an absolute relative error less than ϵ and $\frac{\eta_x}{1-\eta_x} < \epsilon$ we return the approximate value 1 and the upper bound $\frac{\eta_x}{1-\eta_x}$. Note that the upper bound η_x is sometimes called *Mills' ratio,* see Thisted (1988, p. 325), and it is derived here in a very simple way. As we will show, similar bounds are available for other distributions.

In Table 1 we present the results of a simulation comparing the different methods for approximating $F(x)$ and for different choices of n. The first method is labeled H and the second method E. We generated 10^5 standard normal variates and approximated F at these variates with $\epsilon = 10^{-7}$ and the values presented are approximate average CPU times in seconds. We see from this that the methods are roughly comparable and that there is a tremendous improvement in efficiency by using a higher order derivative. For

n	Time H	Time E
0	1.7475	1.4076
1	0.0216	0.0254
2	0.0074	0.0077
3	0.0036	0.0047
4	0.0036	0.0039
5	0.0035	0.0036
6	0.0044	0.0038
8	0.0058	0.0047

Table 1: Average CPU time in seconds for the evaluation of the standard normal distribution function with prescribed error .0000001.

example, the algorithm based on the fifth derivative is 391 times as effiicient as the $n = 0$ case, which corresponds to constructing linear envelopes to the integrand f and integrating these. Of course more efficient algorithms can be constructed for this problem. For example the IMSL routine *anordf* gives a corresponding CPU time of 0.0004 seconds. Still it must remembered that our algorithm also returns upper and lower bounds for the true value of the integral and is derived only using the concavity structure of f.

4.3 The Gamma Function and Distribution Function

We consider constructing an approximation to the gamma function, $\Gamma(\alpha) = \int_0^\infty z^{\alpha-1}e^{-z}\,dz$ where $\alpha > 0$, as another significant test of the utility of the methodology. We note that when $0 < \alpha < 1$ then $\Gamma(\alpha) = \frac{1}{\alpha}\Gamma(\alpha+1)$ and when $\alpha \geq 2$ then $\Gamma(\alpha) = (\alpha-1)\cdots(\alpha - \lfloor\alpha\rfloor + 1)\Gamma(\alpha - \lfloor\alpha\rfloor + 1)$. Therefore we can restrict attention to approximating the gamma function with the argument always in the range $1 \leq \alpha < 2$. In this range $\Gamma(\alpha)$ is always close to 1 and so we avoid problems associated with large values.

We note further that when $1 \leq \alpha$ then $f(z) = z^{\alpha-1}e^{-z}$ is log-concave. The tangent line to $\ln(f)$ at c is given by $\ln(c^{\alpha-1}e^{-c}) + (\frac{\alpha-1}{c} - 1)(z-c)$. For $c > \alpha - 1$ the slope of the tangent line is negative and so we have the bound

$$\begin{aligned}\int_c^\infty z^{\alpha-1}e^{-z}\,dz &\leq \int_c^\infty \exp\left(\ln(c^{\alpha-1}e^{-c}) + (\frac{\alpha-1}{c} - 1)(z-c)\right)dz \\ &= c^\alpha e^{-c}\frac{1}{c-\alpha+1}\end{aligned}$$

on the tail of the integral. We will use this bound to choose c so that the contribution of $\int_c^\infty z^{\alpha-1}e^{-z}\,dz$ to the integral is small and in a moment we discuss how to do this. Note that the same method leads to a bound on the integral over $(0, c)$, and the slope of the tangent is not required to be negative as the interval of integration is compact; namely

$$\begin{aligned}\int_0^c z^{\alpha-1}e^{-z}\,dz &\leq \int_0^c \exp\left(\ln(c^{\alpha-1}e^{-c}) + (\frac{\alpha-1}{c}-1)(z-c)\right)\,dz \\ &= c^{\alpha}e^{-c}\frac{1}{c-\alpha+1}\left(e^{c-\alpha+1}-1\right).\end{aligned}$$

We now suppose that we have chosen c and proceed to approximate the integral $\int_0^c z^{\alpha-1}e^{-z}\,dz$. For the upper and lower envelopes for f on the interval (a, b) we use $z^{\alpha-1}u^{(a,b)}(z)$ and $z^{\alpha-1}l^{(a,b)}(z)$ where $u^{(a,b)}$ and $l^{(a,b)}$ are as in Example 4.1. To integrate these envelopes over (a, b) we need the following recursion for $k \in N_0$; namely

$$\int_a^b z^{\alpha-1}(z-a)^k\,dz = (b-a)^k b^{\alpha-1} - \frac{k}{\alpha-1}\int_a^b z^{\alpha}(z-a)^{k-1}\,dz$$

and note that iterating this leads to a closed form expression for this integral. Therefore it is easy to calculate the upper and lower bounds for $\int_0^c z^{\alpha-1}e^{-z}\,dz$.

We then have that

$$\int_0^c l_m(x)\,dx \leq \Gamma(\alpha) \leq \int_0^c u_m(x)\,dx + c^{\alpha}e^{-c}\frac{1}{c-\alpha+1}$$

and so for an absolute error of ϵ we choose c so that $\delta_c = c^{\alpha}e^{-c}\frac{1}{c-\alpha+1} \ll \epsilon$ and then having chosen n we compound the integration rule, as described in section 2, until $\int_0^c u_m(x)\,dx - \int_0^c l_m(x)\,dx < \epsilon - \delta_c$. It is easy to obtain such a c via bisection. For a relative error in our approximation of no more than ϵ we note that an upper bound on the absolute relative error is given by

$$\left[\frac{\int_0^c u_m(x)\,dx}{\int_0^c l_m(x)\,dx} - 1\right] + \frac{c^{\alpha}e^{-c}\frac{1}{c-\alpha+1}}{\int_0^c l_m(x)\,dx}.$$

Now let α_* be the point in $(1, 2)$ where $\Gamma(\alpha)$ attains its minimum and note that $.8 < \Gamma(\alpha_*) < 1$. To achieve the required bound on the relative error we choose c so that $\delta_c = \frac{\epsilon}{4}$ and then iterate the compounding until both the relative error in the approximation to $\int_0^c z^{\alpha-1}e^{-z}\,dz$ is smaller than $\frac{7}{8}\epsilon$ and $\int_0^c l_m(x)\,dx \geq .5$, both of which are guaranteed to occur under compounding provided $\epsilon/4 < .3$.

The above discussion of the case $1 \leq \alpha < 2$ is modified in obvious ways for the other cases via the formulas given earlier. We note also that for large or very small values of α then relative error is the more sensible error criterion as $\Gamma(\alpha)$ is large. In this situation we can ignore the multiplicative constants as the relative error in the full approximation is given by the relative error in the approximation to the gamma function with its argument in the range $1 \le \alpha < 2$.

The Gamma(α) distribution function is given by

$$F_\alpha(x) = \frac{\int_0^x z^{\alpha-1}e^{-z}\,dz}{\Gamma(\alpha)} = \frac{\int_0^x z^{\alpha-1}e^{-z}\,dz}{\int_0^\infty z^{\alpha-1}e^{-z}\,dz}$$

and there are two integrals that must be approximated in this case. Once again we can reduce the computation to the case $1 \le \alpha < 2$ via

$$F_\alpha(x) = \frac{x^\alpha e^{-x} + \int_0^x z^\alpha e^{-z}\,dz}{\Gamma(\alpha+1)} = \frac{G_\alpha(x)}{\Gamma(\alpha+1)} + F_{\alpha+1}(x)$$

when $0 < \alpha < 1$ and via

$$\begin{aligned} F_\alpha(x) &= \frac{-x^{\alpha-\lfloor\alpha\rfloor}e^{-x}\left[\sum_{k=1}^{\lfloor\alpha\rfloor-1}\prod_{l=1}^{k}\left(\frac{x}{\alpha-\lfloor\alpha\rfloor+l}\right)\right] + \int_0^x z^{\alpha-\lfloor\alpha\rfloor}e^{-z}\,dz}{\Gamma(\alpha-\lfloor\alpha\rfloor+1)} \\ &= \frac{G_\alpha(x)}{\Gamma(\alpha-\lfloor\alpha\rfloor+1)} + F_{\alpha-\lfloor\alpha\rfloor+1}(x) \end{aligned}$$

when $\alpha \ge 2$. Notice that $G_\alpha(x)$ cannot be large but still care must be taken with its evaluation to avoid round-off problems when x is large.

When x is large relative to α then $F_\alpha(x)$ is close to 1. To assess this we obtain a Mill's ratio inequality for the Gamma distribution given by $1 - F_\alpha(x) \le \eta_x$ where

$$\eta_x = \begin{cases} \frac{1}{\Gamma(\alpha_*)}x^\alpha e^{-x}\left(\frac{x}{x-\alpha}+1\right) & if \quad 0 < \alpha < 1 \\ \frac{1}{\Gamma(\alpha_*)}x^\alpha e^{-x}\frac{1}{x-\alpha+1} & if \quad 1 \le \alpha < 2 \\ \frac{1}{\Gamma(\alpha_*)}\frac{1}{(\alpha-1)\cdots(\alpha-\lfloor\alpha\rfloor+1)}x^\alpha e^{-x}\frac{1}{x-\alpha+1} & if \quad \alpha \ge 2. \end{cases}$$

We return the error interval $(1-\eta_x, 1)$ when $\eta_x < \epsilon$ and the criterion is absolute error. Similarly we return $(1-\eta_x, 1)$ when $\frac{\eta_x}{1-\eta_x} < \epsilon$ and the criterion is absolute relative error. Note that the bound we obtained above for $\int_0^c z^{\alpha-1}e^{-z}\,dz$ when $1 \le \alpha < 2$ can be used to determine if x is such that $F_\alpha(x)$ is already close enough to 0 to satisfy the error criterion. For we have $F_\alpha(x) \le \zeta_x$, where

$$\zeta_x = \begin{cases} \frac{1}{\Gamma(\alpha_*)}x^\alpha e^{-x}\left[1+\frac{x}{x-\alpha}\left(e^{x-\alpha}-1\right)\right] & if \quad 0 < \alpha < 1 \\ \frac{1}{\Gamma(\alpha_*)}x^\alpha e^{-x}\frac{1}{x-\alpha+1}\left(e^{x-\alpha+1}-1\right) & if \quad 1 \le \alpha < 2 \\ \frac{1}{\Gamma(\alpha_*)}\frac{1}{(\alpha-1)\cdots(\alpha-\lfloor\alpha\rfloor+1)}x^\alpha e^{-x}\frac{1}{x-\alpha+1}\left(e^{x-\alpha+1}-1\right) & if \quad \alpha \ge 2. \end{cases}$$

n	Time
0	6.0132
1	0.2598
2	0.1584
3	0.0810
4	0.0714
5	0.0708
6	0.0714
7	0.0744
10	0.0882

Table 2: Average CPU time in seconds for the evaluation of a Gamma distribution function with prescribed error .00001.

Now suppose that $1 \leq \alpha < 2$. Then approximating $F_\alpha(x)$ requires approximating $\Gamma(\alpha)$ and $\int_0^x z^\alpha e^{-z}\,dz$. It makes sense to include x, provided that it is not too large relative to α as determined above, in the partition formed to approximate $\Gamma(\alpha)$. Then both integrals can be simultaneously approximated with no more work involved than approximating the gamma function. For the case where $0 < \alpha < 1$ the upper and lower bounds for $\Gamma(\alpha+1)$ lead to lower and upper bounds for $G_\alpha(x)/\Gamma(\alpha+1)$ and these are combined with the lower and upper bounds for $F_{\alpha+1}(x)$ to give lower and upper bounds for $F_\alpha(x)$. We proceed similarly for the case where $\alpha \geq 2$.

We see then that we have specified a complete methodology for approximating the gamma function or gamma distribution function with prescribed absolute or relative error being attained in our approximations. In Table 2 we present some average computation times for Gamma(α) distribution functions based on 10^5 values obtained by generating α uniformly in (0,50) and then generating x from the Gamma(α) distribution. Again we see a tremendous improvement in efficiency by going to higher order derivatives. Correspondingly the average computation time for the IMSL routine *gamdf* was about 100 times faster than the fastest time we recorded so our current routine is not very competitive. We have not , however, tried to optimize our algorithm as our intent here is only to show that the method of the paper can be used to design an effective algorithm for a broad family of distribution functions. Also we recall that our algorithm is returning a guaranteed error bound.

4.4 Makeham's Distribution Function

The density function for this distribution is given by

$$f(z) = (\alpha + \beta\gamma^z)\exp(-\alpha z - \frac{\beta}{\ln(\gamma)}(\gamma^z - 1))$$

where $\beta > 0, \gamma > 1, \alpha > -\beta$ and $z \geq 0$. It is not hard to show that $f(z)$ is log-concave when either $\alpha < 0$ or, if $\alpha \geq 0$ when

$$z \geq \frac{\ln\left[\max\left(\frac{-\alpha+\sqrt{\alpha\ln(\gamma)}}{\beta}, 1\right)\right]}{\ln(\gamma)}.$$

Further the tangent to $\ln(f(z))$ at x has a negative sign whenever $\ln(\gamma) < 4\alpha$ or, if this inequality doesn't hold, when

$$x > \frac{1}{2\beta}\left[(\ln(\gamma) - 2\alpha) + \ln(\gamma)\sqrt{\ln(\gamma) - 4\alpha}\right].$$

So if x is in the log-concave right tail then Mill's ratio inequality for this distribution is given by

$$1 - F(x) \leq f(x)\left[\alpha + \beta\gamma^x - \ln(\gamma)\frac{\beta\gamma^x}{\alpha + \beta\gamma^x}\right]^{-1}$$

and we can use this to determine whether or not x is so large that we can return the approximation 1 for $F(x)$.

Putting $\alpha^* = \alpha/\ln(\gamma)$and $\beta^* = \beta/\ln(\gamma)$ and making the transformation $y = \beta^*\gamma^z$ we have that the density of y is

$$g(y) = (\beta^*)^{\alpha^*} e^{\beta^*}(\alpha^* + y)\, y^{-\alpha^*-1}e^{-y}$$

for $y > \beta^*$. Then we have that

$$F(x) = \int_{\beta^*}^{\beta^*\gamma^x} g(y)\,dy.$$

To evaluate the integral of g over (a, b) we use the upper and lower envelopes

$$\begin{aligned} u(y) &= (\beta^*)^{\alpha^*} e^{\beta^*}(\alpha^* + y)\, y^{-\alpha^*-1}u^{(a,b)}(y) \\ l(y) &= (\beta^*)^{\alpha^*} e^{\beta^*}(\alpha^* + y)\, y^{-\alpha^*-1}l^{(a,b)}(y) \end{aligned}$$

and note that the integrals of these functions over (a, b) can be evaluated as in Example 4.3. So with a small modification the algorithm for the Gamma distribution function can be used here as well.

4.5 Bivariate Student Probabilities of Rectangles

The Student$_2(\lambda)$ probability content of the rectangle $[a,b]$ is given by

$$P([a,b]) = \frac{\lambda}{2\pi}\int_{[a,b]} f(x,y)\,dx\,dy$$

where $f(x,y) = \left(1+\frac{x^2+y^2}{\lambda}\right)^{-\frac{\lambda+2}{2}} = h(g(x,y))$ with $g(x,y) = x^2+y^2$ and $h(t) = (1+\frac{t}{\lambda})^{-\frac{\lambda+2}{2}}$ for $t \geq 0$. For the integration we employ upper and lower envelopes to $h^{(n)}$ on $[c,d]$ and note that $c = \min\{x^2+y^2 : (x,y) \in [a,b]^*\}$ and $d = \max\{x^2+y^2 : (x,y) \in [a,b]^*\}$. Also we have that

$$h^{(n)}(t) = \frac{(-1)^n}{\lambda^n}\left(\frac{\lambda+2}{2}\right)\cdots\left(\frac{\lambda+2}{2}+n-1\right)\left(1+\frac{t}{\lambda}\right)^{-\frac{\lambda+2}{2}-n}$$

and from this we see that the derivatives of h are alternately concave and convex everywhere. Note that an appropriate generalization of Lemma 7, as we generalized Lemma 3, guarantees the success of this approach.

For the approximation we must first reduce integration over R^2 to a compact region. To do this we make the transformation $(x,y) \rightarrow (r,\theta)$ given by $x = r\cos(\theta), y = r\sin(\theta)$ and therefore

$$\frac{\lambda}{2\pi}\int_{\{(x,y):x^2+y^2>c\}} f(x,y)\,dx\,dy = \lambda\int_c^\infty r\left(1+\frac{r^2}{\lambda}\right)^{-\frac{\lambda+2}{2}} dr.$$

It is easy to show that $k(r) = \left[r\left(1+\frac{r^2}{\lambda}\right)^{-\frac{\lambda+2}{2}}\right]^p$ is convex for large r when $p = -1/(\lambda+2)$. Then $k(c) + k'(c)(r-c) \leq k(r)$ for all $r \geq c$ with $k'(c) > 0$, provided c is large enough, and since the transformation $T(x) = x^p$ is strictly decreasing we have that

$$\begin{aligned}
\lambda\int_c^\infty k^{\frac{1}{p}}(r)\,dr &\leq \lambda\int_c^\infty T^{-1}\left(k(c)+k'(c)(r-c)\right)\,dr \\
&= \lambda\int_c^\infty \left(k(c)+(k(c))'(r-c)\right)^{\frac{1}{p}}\,dr = \frac{-\lambda}{\left(\frac{1}{p}+1\right)}\frac{k^{\frac{1}{p}+1}(c)}{k'(c)} \\
&= \lambda^2\frac{\lambda+2}{\lambda+1}\left(1+\frac{c^2}{\lambda}\right)^{-\frac{1}{2}\lambda}\frac{\frac{c^2}{\lambda}}{\frac{c^2}{\lambda}(\lambda+1)-1}. \qquad (6)
\end{aligned}$$

It is easy to show that $k'(c) > 0$ provided $c > \sqrt{\frac{\lambda}{\lambda+1}}$. Note that (6) is a Mill's ratio inequality for the bivariate Student. For an appropriate choice

n	Time
2	0.053
4	0.040
6	0.030
8	0.031
10	0.035
12	0.041

Table 3: Average CPU time in seconds for the evaluation of the probability content, with respect to a standard bivariate Student distribution, of a rectangle with prescribed error .00005.

of c we then replace $[a, b]$ by $[a, b] \cap [(-c, c), (-c, c)]$ and use compounding on this rectangle. In Table 3 we present average computation times based on a simulation where we generated 10^3 rectangles by generating pairs of values from a standard bivariate normal and then generating λ uniformly in (0,30). Due to the long computation times we haven't bothered to record the $n = 0$ and $n = 1$ cases.

While we have presented the calculations for the standard bivariate Student it is possible to easily generalize this to the general bivariate Student as this only requires that we be able to integrate bivariate polynomials over parallelepipeds and this can be carried out exactly. Similarly the approach can be generalized to higher dimensions although there are obviously some computational limits on this. Bohrer and Schervish (1981) in their development of an algorithm for the contents of rectangles for the bivariate normal, mention dimension 5 as about the limit for their algorithm. We will systematically investigate the dimensional limits to our approach elsewhere.

5 Conclusions

We have presented a class of algorithms useful for computing approximations to integrals with exact error bounds with respect to absolute or relative error. The utility of the algorithms has been demonstrated by their application to a number of integration problems. While our algorithms may lose in a speed competition in some integration problems with highly-developed algorithms, they have the virtue of returning exact error bounds. Further, and perhaps most importantly, the methodology of this paper presents a set of techniques that a practitioner can use to develop useful algorithms when confronted with non-standard integration problems and these do not typically require extensive study of properties of the integrand. Further research will consider the use of these techniques to evaluate various multidimensional distribution functions and extend the approach to non-rectangular domains.

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