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# COMPUTING TAIL PROBABILITIES BY NUMERICAL FOURIER INVERSION: THE ABSOLUTELY CONTINUOUS CASE

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*Abstract:* The numerical computation of $P\{X > x\}$ can be accomplished in a variety of ways. An appealing class of methods may be derived from the contour integral connecting $P\{X > x\}$ and its Fourier representation. Statisticians have largely focused on deriving saddlepoint approximations for this contour integral. The accuracy of such approximations is generally understood in vague terms only and, perhaps more importantly, is rarely under user control. Numerical integration of the contour integral has received considerably less attention, particularly in the statistics literature. The focus of this paper is on the use of the trapezoidal rule applied to said contour integral along an appropriate path. An exponential bound on the approximation (i.e., discretization) error of the trapezoidal rule as a function of the quadrature node spacing is obtained using results of Stenger (1993). This bound is used in developing a reliable non-iterative method of selecting the trapezoidal rule spacing that guarantees control of the approximation error. The epsilon algorithm is used to accelerate the calculation of the tail of the infinite series that results upon applying the trapezoidal rule to the inversion integral. The resulting "automatic" methodology is shown to produce extremely accurate results in a diverse set of problems.

*Key words and phrases:* Analytic function, characteristic function, epsilon algorithm, saddlepoint recentering, sinc quadrature.

## 1. Introduction

The "exact" calculation of a tail probability $P\{X > x\}$ can be accomplished in a variety of ways, including direct computation through a closed form expression, numerical integration of a known probability density, summation of point probabilities, and so on. In principle, tail probabilities may also be computed via well-known Fourier inversion theorems linking $P\{X > x\}$ to the characteristic function of $X$; see, for example, Kawata (1972) or Lukacs (1970). These inversion theorems have potential value in cases where the characteristic function is easy to obtain and simple expressions for the associated tail probability are not. For example, as pointed out by Mehta, Senchaudhuri and Patel (1998), numerous problems in exact conditional inference are well-suited to such methods since the

characteristic function is either known or can be computed easily; in contrast, the direct computation of a tail probability can require enormous computational effort.

In statistics, the Fourier representation of a tail probability has primarily been exploited through saddlepoint approximation and related asymptotic methods; see Strawderman (2000) for a selective review. Widely cited sources detailing statistical uses of these approximations include Barndorff-Nielsen and Cox (1989, 1994), Daniels (1954, 1983, 1987), Jensen (1995), Kolassa (1997), Lugannani and Rice (1980) and Field and Ronchetti (1990). Excellent results have been achieved in the case where $X$ represents a sum of independent and identically distributed random variables. Outside of this comparatively straightforward setting, the conditions required for the validity of these asymptotic approximations become substantially more difficult to write down. In all cases, the approximation error is only vaguely understood and typically depend on factors (e.g., sample size) that are not under user control. These factors are significant obstacles to the trustworthy, routine use of saddlepoint approximations.

Numerical integration of the Fourier inversion integral has received considerably less attention from statisticians. Abate and Whitt (1992) provide an extensive and interesting discussion of various methods for numerical transform inversion, the focus primarily being applications in probability involving distributions supported on the positive real line. Later refinements of this work include Abate and Whitt (1995) and Abate, Choudhury and Whitt (1999). Most of the quadrature-based methods considered in these papers are "Fourier series" (i.e., trapezoidal rule) approximations. Waller, Turnbull and Hardin (1995) provide a more limited, statistically oriented review of similar methods and in particular illustrate the use of one method previously described in Böhman (1975). Together, the respective reference lists of these two papers covers most of the work by statisticians on numerical transform inversion. The attraction of numerical quadrature is apparent: in principle, an exact answer can be obtained to any specified level of precision, the resulting error being largely controlled by the number and placement of quadrature nodes. However, the problem is also beset with numerical difficulties, most of which can be traced to the rapidly oscillating Fourier integrand (Davis and Rabinowitz (1984)). A recent survey of existing numerical quadrature schemes for oscillatory integrands can be found in Krommer and Ueberhuber (1998).

The Fourier integrands arising in the representation of tail probabilities have properties that are neither exploited by existing methods for transform inversion nor by more general quadrature schemes for oscillatory integrands. For example, when the moment generating function (MGF) of the random variable of interest exists, the corresponding characteristic function and resulting Fourier

integrand are both analytic. The analytic behavior of the integrand has a number of useful implications. For example, the path of integration in the contour integral may be altered, allowing substantial flexibility; an important choice of path is that which passes through a saddlepoint (e.g., Rice (1980) and Helstrom (1983)). Upon such path modification, the resulting inversion integral reduces to the Fourier transform of an analytic function, opening up a number of new computational possibilities. Using the results of Stenger (1993), it is proved that the trapezoidal rule provides an extraordinarily accurate approximation to the tail probability inversion integral. This approximation suffers from an unfortunate computational drawback: it requires the summation of an infinite series. It will be shown, however, that this series can be accurately summed using a modest number of terms provided "convergence acceleration" is also employed. This paper exploits these observations in order to derive an effective quadrature rule for tail probability computations involving differentiable CDFs supported on any subset of the real line. The method to be described applies to the computation of almost any univariate tail probability, the main proviso being existence of the MGF (a condition also required for saddlepoint methods).

In essential respects the conclusions of this paper reflect those of Abate and Whitt (1992): the trapezoidal rule, combined with convergence acceleration, creates a powerful and effective tool for computing tail probabilities by numerical inversion. However, the implementation to be described here differs from the methods described in Abate and Whitt (1992). These differences stem primarily from the assumed existence of the MGF, which has important implications for the mathematical behavior of the characteristic function. One particularly useful consequence is a simple exponential bound on the approximation error of the trapezoidal rule, yielding an easy non-iterative method for selecting an appropriate spacing. The error bound depends primarily on the MGF and path of integration selected, and shows that the latter can have important implications for determining both the number of and spacing between quadrature nodes. In contrast, the error bounds for most of the quadrature methods detailed in Abate and Whitt (1992) are derived via the Poisson summation formula. For general probability distributions, these bounds require information about the tail behavior of the CDF (i.e., the quantity being computed) in order to determine an appropriate choice of spacing; however, it is possible to avoid this requirement in the case of probability distributions supported on the positive real line (Abate and Whitt (1992, 1995)). The existence of the MGF also leads to asymptotic regularity of the zero pattern in the Fourier integrand. This regularity is valuable because it substantially increases the chances for successful convergence acceleration. For these purposes, the method of choice in Abate and Whitt (1992) is Euler summation. The epsilon algorithm is used here (e.g., Brezinski and Redivo

Zaglia (1991)), and significantly outperforms Euler summation in the examples considered in Section 5.

The remainder of this paper will proceed as follows. In Section 2, the inversion integral representation of a tail probability for an absolutely continuous random variable is reviewed. It is shown that this integral may be written as a standard Fourier transform. In Section 3.1, some theory for trapezoidal rules applied to general Fourier transforms is reviewed. In Section 3.2, this theory is used to obtain an exponential bound on the approximation error of the trapezoidal rule when applied to the tail probability inversion integral. Section 4 provides one possible implementation of this theory. In Section 5, the proposed methodology is applied to some problems previously considered in the literature. The paper closes with a discussion in Section 6.

## 2. Fourier Representation of Tail Probabilities

### 2.1. Preliminaries

Let $X$ be a random variable with cumulative distribution function $F(\cdot)$. For example, $X$ might represent the convolution of several independent random variables; alternatively, $X$ might be the sufficient statistic for a univariate parameter of interest in a generalized linear model (e.g., see Davison (1988)). For $t \in \mathbb{R}$, suppose the MGF $M(t) = E[e^{tX}]$ exists for $t \in \mathcal{E}$, where $\mathcal{E}$ is an open interval containing $t = 0$. Let $K(t)$ denote the associated cumulant generating function (CGF). Finally, let the characteristic function of $X$ be $\xi(t) = E[e^{itX}]$, where $i = \sqrt{-1}$ and $\xi(t) = M(it)$.

Definitions of these quantities valid for complex-valued arguments will also be required. Let $z = x + iy \in \mathbb{C}$, where $x, y \in \mathbb{R}$ and $\mathbb{C}$ denotes the complex plane. Let $\Re(z) = x$ and $\Im(z) = y$ respectively denote the real and imaginary parts of $z$. Let $D_d = \{z \in \mathbb{C} : z = x + iy, x \in \mathbb{R}, |y| < d\}$ denote an infinite strip of width $2d$ containing the real axis $\mathbb{R}$. Define the complex-valued function $\xi(z) = E[e^{izX}] = M(iz)$, and observe that the characteristic function is recovered for $\Im(z) = 0$. Importantly, the existence of $M(\cdot)$ implies $\xi(z) = M(-y + ix)$ is analytic for $z \in D_d$ (Lukacs (1970, Theorem 7.1.1)). If $X$ has bounded support, then $D_d$ becomes the complex plane $\mathbb{C}$ (i.e., $\xi(z)$ is entire) (Lukacs (1970, Theorem 7.2.3)). Otherwise, the strip of regularity takes the form $-\alpha < \Im(z) < \beta$ for $\alpha, \beta > 0$, where $-i\alpha$ and $i\beta$ are the singularities of $\xi(z)$ closest to the origin (Lukacs (1970, Theorem 7.1.1)).

### 2.2. The absolutely continuous case

In the case where $X$ is absolutely continuous, there are numerous forms of the so-called "inversion integral" for $P\{X > x\}$; see, for example, Abate and

Whitt (1992). When the MGF exists, a general form providing a useful starting point is the following:

$$P\{X > x\} = \mathcal{H}(-c) + \frac{e^{\nu(c)}}{2\pi i} \int_{c-i\infty}^{c+i\infty} z^{-1} \exp\{\nu(z) - \nu(c)\}\, dz, \tag{1}$$

where $c \in \mathcal{E}$, $\nu(z) = K(z) - xz$ for $z \in \mathbb{C}$, and $\mathcal{H}(w)$ respectively equals 0, 1/2, or 1 if $w < 0$, $w = 0$, or $w > 0$. Saddlepoint approximations for this contour integral may be derived under suitable conditions. Typically, one selects $c = \widehat{u}_x$, where $K'(\widehat{u}_x) = x$; doing so,

$$P\{X > x\} = \mathcal{H}(-\widehat{u}_x) + \frac{e^{\nu(\widehat{u}_x)}}{2\pi i} \int_{\widehat{u}_x-i\infty}^{\widehat{u}_x+i\infty} z^{-1} \exp\{\nu(z) - \nu(\widehat{u}_x)\}\, dz. \tag{2}$$

As $\widehat{u}_x \to 0$ (i.e., as $x \to E[X]$), a pole occurs in the integrand on the right-hand side of (2) at $z = 0$. In general, solutions for this problem have been devised with a view towards generating valid asymptotic expansions; see, for example, Daniels (1987) and Kolassa (1997). However, in view of Cauchy's theorem (see Bak and Newman (1996)) the choice of $c$ is arbitrary and other selections are possible. Helstrom (1983) proposed setting $c = \bar{u}_x$, where

$$\nu'(\bar{u}_x) - \bar{u}_x^{-1} = 0. \tag{3}$$

The solution to (3) maximizes the entire integrand in (2) (i.e., as opposed to just the exponential term). Taking the path of integration through $\bar{u}_x$ is less desirable from an asymptotic point of view because of the resulting difficulties associated with applying Watson's Lemma; for related discussion see Section 5.6 of Kolassa (1997). However, it is an interesting and useful choice because (i) $\bar{u}_x \approx \widehat{u}_x$ as $x$ moves towards the limits of the support of $X$, maintaining whatever benefits are afforded by saddlepoint methods for "extreme" $x$; and (ii), the solution to (3) remains bounded away from zero as $x \to E[X]$, resolving the potential numerical instability associated with using $\widehat{u}_x$ for $x$ near $E[X]$.

The integral (1) with $c = \bar{u}_x$ will now be expressed in a less familiar form. Specifically, parameterizing the path in $\mathbb{C}$ as $\bar{u}_x + it$ for $t \in \mathbb{R}$, one may write

$$P\{X > x\} = \mathcal{H}(-\bar{u}_x) + \frac{e^{\nu(\bar{u}_x)}}{2\pi} \int_{-\infty}^{\infty} g_x(t) e^{-ixt} dt, \tag{4}$$

where

$$g_x(t) = \frac{\exp\{K(\bar{u}_x + it) - K(\bar{u}_x)\}}{\bar{u}_x + it}. \tag{5}$$

The integral appearing in (4) takes the form of an (inverse) Fourier transform of the complex-valued function $g_x(t)$. Consequently, any quadrature rule appropriate for a Fourier transform can in principle be used to compute $P\{X > x\}$. The

focus in this paper will be on the trapezoidal rule, which is explored in detail in the remaining sections. Notably, $g_x(t)e^{-ixt}$ generally has both a nonzero real and imaginary part, the latter being an odd function of $t$. It follows that (4) may be expressed in terms of $\Re\{g_x(t)e^{-ixt}\}$ only. However, this fact will not be exploited until later.

**Remark A.** In deriving (4), the path of integration is a straight line passing through the saddlepoint $\bar{u}_x$. An important alternative choice is to integrate along a path of steepest descent. This is not done because it is typically impossible to characterize these paths explicitly. The "saddlepoint approximation" is an asymptotic approximation to (2). In statistical applications, it is usually derived by using a quadratic approximation to the path of steepest descent in a neighborhood of the saddlepoint $\widehat{u}_x$. Generally, the region on which this approximation is valid is not specified, and contributions to (2) of the integrand outside of this region are thus considered as part of the error term. For tail probabilities involving a mean of i.i.d. random variables, these errors vanish at a geometric rate depending on the sample size. This is not necessarily true more generally, and ignoring them can produce substantial inaccuracy.

## 3. Trapezoidal Rules for Tail Probabilities

### 3.1. The importance of smoothness

A trapezoidal rule is typically derived as the exact integral of a piecewise linear approximation to a given integrand. Assuming only that the integrand has two continuous derivatives, this derivation leads one to conclude that the associated approximation error is $O(h^2)$, where $h$ is the spacing between quadrature nodes. Interesting alternative derivations of the trapezoidal rule exist that better highlight the role of integrand smoothness and in particular substantially refine the usual $O(h^2)$ error bound. Though several versions of such results are available in the literature (e.g., see Butzer and Stens (1983)), of importance to this paper is the fact that the trapezoidal rule may be derived as the exact integral of the Whittaker cardinal (or sinc) function expansion of the integrand; see, for example, Stenger (1993). For analytic integrands (i.e., differentiable when considered as a function of $z \in \mathbb{C}$), contour integration may be used to show that the approximation error vanishes exponentially fast. The following result establishes the rate of convergence of the trapezoidal rule when applied to the Fourier transform of an analytic function; the error bound refines that given in Theorem 3.3.1 of Stenger (1993):

**Theorem 1.** *For $d > 0$, let $D_d = \{z \in \mathbb{C} : z = x + iy, x \in \mathbb{R}, |y| < d\}$, and define $B(D_d)$ to be the set of functions $f$ satisfying*
(i) *For $z \in D_d$, $f(z)$ is analytic,*

(ii) $\int_{-d}^{d} |f(t+iy)|dy \to 0$ *as* $|t| \to \infty$,
(iii) $\mathcal{N}_\omega(f, D_d) < \infty$, *where*

$$\mathcal{N}_\omega(f, D_d) = \lim_{y \to d-} \int_{-\infty}^{\infty} \left[ e^{\omega d} |f(t-iy)| + e^{-\omega d} |f(t+iy)| \right] dt. \tag{6}$$

*Suppose* $f \in B(D_d)$. *Then, for* $0 < h < \frac{2\pi d}{\log 2}$ *and* $|\omega| < \pi h^{-1}$,

$$\left| \int_{-\infty}^{\infty} f(t) e^{i\omega t} dt - h \sum_{k=-\infty}^{\infty} f(kh) e^{i\omega kh} \right| \leq 2\mathcal{N}_\omega(f, D_d) \exp\{-2\pi d/h\}.$$

This result says that the approximation error of the trapezoidal rule vanishes exponentially fast as $h \to 0$ for functions $f(\cdot)$ that satisfy certain differentiability and integrability conditions when considered as a function of $z \in \mathbb{C}$. The convergence rate is affected by transform ordinate (i.e., $|\omega|$) and the width of the region in which $f$ is analytic (i.e., $d$). In the next section, this result is used to bound the approximation error of the trapezoidal rule when applied to (4).

### 3.2. The approximation error for tail probabilities

Provided the required conditions are met, Theorem 1 applies directly to the integral appearing in (4) upon making the identifications $\omega = -x$ and $f(t) = g_x(t)$, where $g_x(t)$ is given in (5). The following result, proved in Appendix, provides sufficient conditions under which Theorem 1 applies to the computation of (4).

**Theorem 2.** *Let* $X$ *be an absolutely continuous random variable with CDF* $F(\cdot)$ *and density* $F'(\cdot)$. *Suppose* $M(t) = \exp\{K(t)\} < \infty$ *for* $t \in \mathcal{E}$, *where* $\mathcal{E}$ *is an open interval containing* $t = 0$. *Let* $\delta = \min\{|s| : s \notin \mathcal{E}\} > 0$ *and, for a given* $x \in \mathbb{R}$, *suppose* $\min\{F(x), 1 - F(x)\} > 0$. *Finally, let* $\beta$ *and* $r > 0$ *be such that* $M(\beta) < \infty$ *and*

$$\frac{M(\beta + is)}{M(\beta)} = O(s^{-r}) \tag{7}$$

*as* $|s| \to \infty$. *Then,* (i)-(iii) *of Theorem* 1 *are satisfied by* $g_x(z)$ *for* $z \in D_{d^\star}$, *where*

$$\begin{aligned} &1.\ \text{for } \mathcal{E} = \mathbb{R},\ 0 < d^\star < |\bar{u}_x|, \\ &2.\ \text{for } \mathcal{E} = (-\infty, \delta),\ 0 < d^\star < \min\{|\delta - \bar{u}_x|, |\bar{u}_x|\}, \\ &3.\ \text{for } \mathcal{E} = (-\delta, \infty),\ 0 < d^\star < \min\{|\delta + \bar{u}_x|, |\bar{u}_x|\}, \\ &4.\ \text{for } \mathcal{E} \text{ a bounded interval, } 0 < d^\star < \min\{|\delta + \bar{u}_x|, |\delta - \bar{u}_x|, |\bar{u}_x|\}. \end{aligned} \tag{8}$$

*Moreover, with* $h = \pi/\Delta$, $\Delta > \max\{|x|, \log 2/(2d^\star)\}$, *and*

$$\mathcal{I}_x(h) = \frac{h}{2} \sum_{k=-\infty}^{\infty} g_x(kh) e^{-ixkh}, \tag{9}$$

*the following error bound holds:*

$$\left|P\{X > x\} - \left[\mathcal{H}(-\bar{u}_x) + \frac{e^{\nu(\bar{u}_x)}}{\pi}\mathcal{T}_x(h)\right]\right| \leq \eta(\Delta, x),$$

*where* $\eta(\Delta, x) = \pi^{-1}\mathcal{N}_x(g_x, D_{d^\star})\exp\{\nu(\bar{u}_x) - 2\Delta d^\star\}$ *and* $\mathcal{N}_x(g_x, D_{d^\star})$ *is defined as in* (6).

The error $\eta(\Delta, x)$ decays exponentially as $\Delta \to \infty$ (i.e., $h \to 0$). This observation is useful precisely because $h = \pi/\Delta$ is the main parameter under user control. In particular, to bound $\eta(\Delta, x)$ above by $\epsilon_a > 0$, one must only select $\Delta$ satisfying $\eta(\Delta, x) < \epsilon_a$. This requires specifying $d^\star$ and computing $\mathcal{N}(g_x, D_{d^\star})$, problems dealt with in the next section.

**Remark B.** The assumptions that $X$ has a probability density and MGF require no discussion. The key assumption is (7), which requires that the characteristic function of the exponentially tilted density $q_\beta(u) = e^{\beta u}F'(u)/M(\beta)$ decay to zero at least algebraically. This relatively weak condition holds with $r = 1$ provided $F''(\cdot)$ exists and is integrable; see also Lemma 6.2.1 of Bleistein and Handelsman (1975). However, (7) holds under much weaker conditions; see, for example, Lemma 12.3 of Olver (1974) or Theorem 1 of Wong ((1989), §IV.2). Finally, it is noted that (7) can be guaranteed by considering instead the CDF of the convolution $X + Z_\sigma$, where $Z_\sigma \sim N(0, \sigma^2)$ and $X \perp Z_\sigma$. In this case, Theorem 2 provides an accurate approximation to the CDF of $X + Z_\sigma$; the accuracy of the latter as an approximation to the CDF of $X$ depends primarily on $\sigma$ and, to a lesser extent, $F(\cdot)$.

**Remark C.** Theorem 2 continues to hold with $\bar{u}_x$ replaced by any other constant $c$, provided $c$ is restricted to be interior to $\mathcal{E}$. This observation has some useful practical implications. Typically, $\bar{u}_x$ approaches the boundaries of $\mathcal{E}$ as $x$ approaches the limits of the support of $X$; see, for example, Daniels ((1954), §6). In this situation and when $\delta < \infty$ (i.e., $\mathcal{E}$ is either semi-infinite or finite), it can happen that $d^\star \to 0$. To see this, suppose $\bar{u}_x > 0$ (i.e., $x > E[X]$) and $\mathcal{E} = (-\infty, \delta)$ where $\delta < \infty$. Then, $\min\{|\delta - \bar{u}_x|, |\bar{u}_x|\} \to 0$ and hence $d^\star \to 0$ as $\bar{u}_x \to \delta$ (i.e., as $x$ approaches the upper bound of the support of $X$). This is problematic because the error bound $\eta(\Delta, x)$ depends on $d^\star$ through $\mathcal{N}_x(g_x, D_{d^\star})\exp\{-2d^\star\Delta\}$. For example, if $\mathcal{N}_x(g_x, D_{d^\star})$ changes slowly as $d^\star \to 0$, $\Delta$ will typically need to be increased (i.e., $h$ decreased) in order to maintain $\eta(\Delta, x)$ at a given level. Since decreasing $h$ tends to increase the number of quadrature nodes required, this can adversely affect computation. Intuitively, bounding $\bar{u}_x$ away from the boundaries of $\mathcal{E}$ should alleviate such difficulties. However, as the discussion in Section 4.1 will reveal, this is not quite sufficient; one must also be careful in fixing the value of $d^\star$. One simple solution addressing these issues is given in Lemma 1.

In addition to approximation error, one must also consider the error incurred by truncating the infinite sum (9). This is important in probability computations because the integrand $g_x(\cdot)$ generally decays to zero at a rate governed by the number of integrable derivatives of $F$ on $\mathbb{R}$ (e.g., Feller (1971, Lemma 4, p.514)). When the number of such derivatives is small, the resulting slow rate of decay may require the computation of a large number of terms in (9) in order to attain a desired level of accuracy. It is possible to place conservative bounds on the truncation error under minimal assumptions; see, for example, Abate and Whitt ((1992), §6). These bounds typically yield inefficient quadrature schemes, and a more adaptive approach often proves beneficial. In Section 4.4 a hybrid approach is proposed that involves selecting an initial truncation point based on properties of the integrand. The initial approximation is then improved using convergence acceleration techniques.

## 4. Implementation

The next three sections describe one implementation of the theory of the previous section. It is assumed that an approximation to $P\{X > x\}$ to within $\epsilon_{tot} > 0$ is desired. Previous discussion implies $\epsilon_{tot} = \epsilon_t + \epsilon_a$, where $\epsilon_a > 0$ denotes approximation error and $\epsilon_t > 0$ denotes truncation error; here it is assumed that $\epsilon_a = \epsilon_t = \epsilon_{tot}/2$. The methodology below is guaranteed to control the level of approximation error. However, guaranteeing control of the truncation error $\epsilon_t$ is considerably more difficult, particularly if computational efficiency is of concern. One method for dealing with this problem is discussed in Section 4.4. While the proposed method is unable to provide an explicit guarantee, the results of Section 5 show that it works extremely well.

As discussed in Remark C, a modified version of $\bar{u}_x$ may prove useful in handling certain numerical problems. Section 4.1 details a simple but effective proposal. Subsequent to this modification, the essential steps for implementing the theory of Section 3.2 are then: (i) determine an approximation to $\mathcal{N}_x(g_x, D_{d^\star})$; (ii) select an appropriate spacing $h = \pi/\Delta$; and (iii), accurately compute (9). The first two relate to the control of approximation error; the last primarily reflects control of the truncation error. Sections 4.2 and 4.3 below contain the major supporting details for Steps 1 and 2; Section 4.4 contains the key details required for understanding how Step 3 will be handled. The main computational algorithm is then summarized in Section 4.5.

### 4.1. A modification of $\bar{u}_x$

The discussion following Theorem 2 suggests that the magnitude of $d^\star$ plays a significant role in determining $\Delta$, hence $h$ and possibly the number of quadrature nodes required for the accurate computation of (9). These difficulties may arise

when the set $\mathcal{E}$ is bounded above or below (or both). Since $\mathcal{E}$ is dictated by the problem under consideration, alleviating the aforementioned difficulties evidently requires modification of $\bar{u}_x$ or, equivalently, the path of integration; Lemma 1 provides one possible choice.

**Lemma 1.** *Let* $\kappa = I\{\bar{u}_x > 0\}$. *Then Theorem* 2 *continues to hold with* $\bar{u}_x$ *replaced by* $\bar{\bar{u}}_x$ *and* $d^\star = |\bar{\bar{u}}_x|/2$, *where*

1. *for* $\mathcal{E} = \mathbb{R}$, $\bar{\bar{u}}_x = \bar{u}_x$,
2. *for* $\mathcal{E} = (-\infty, \delta)$, $\bar{\bar{u}}_x = \kappa \min\{\bar{u}_x, \frac{\delta}{2}\} + (1-\kappa)\bar{u}_x$,
3. *for* $\mathcal{E} = (-\delta, \infty)$, $\bar{\bar{u}}_x = (1-\kappa)\max\{\bar{u}_x, -\frac{\delta}{2}\} + \kappa\bar{u}_x$,
4. *for* $\mathcal{E}$ *a bounded interval,* $\bar{\bar{u}}_x = (1-\kappa)\max\{\bar{u}_x, -\frac{\delta}{2}\} + \kappa\min\{\bar{u}_x, \frac{\delta}{2}\}$.

*Moreover,* $\mathcal{N}_x(g_x, D_{d^\star}) = \int_{-\infty}^{\infty}[e^{-xd^\star}|g_x(t - id^\star)| + e^{xd^\star}|g_x(t + id^\star)|]dt$.

The proof of Lemma 1 is identical to Theorem 2 and is omitted. No modification to the path of integration is required if $\mathcal{E} = \mathbb{R}$ since $\bar{u}_x$ is bounded away from zero. In the remaining cases, $\bar{\bar{u}}_x$ is bounded away from the finite boundaries of $\mathcal{E}$, preventing the bounds on $d^\star$ in (8) from converging to zero.

With $\bar{\bar{u}}_x$ as defined, the restrictions on $d^\star$ detailed in (8) can be further reduced to the single constraint $0 < d^\star < |\bar{\bar{u}}_x|$. The reason Lemma 1 sets $d^\star$ to be one half the distance to $|\bar{\bar{u}}_x|$ is to avoid further numerical problems when computing $\mathcal{N}_x(g_x, D_{d^\star})$. In particular, $\mathcal{N}_x(g_x, D_{d^\star})$ can still grow without bound as $d^\star \to |\bar{\bar{u}}_x|$, resulting in problems similar to those discussed in Remark C. The remainder of this paper employs $\bar{\bar{u}}_x$ in place of $\bar{u}_x$ and $d^\star = \bar{\bar{u}}_x/2$.

### 4.2. Approximating $\mathcal{N}_x(g_x, D_{d^\star})$

In order to select $\Delta$ to bound the approximation error of the trapezoidal rule, the constant $\mathcal{N}_x(g_x, D_{d^\star})$ of Lemma 1 must be computed. However, since $\mathcal{N}_x(g_x, D_{d^\star})$ appears as part of an upper bound, it need not be computed to a high level of precision. Below, an approximation to $\mathcal{N}_x(g_x, D_{d^\star})$ is obtained that significantly facilitates its computation.

Define for suitable $\alpha$ the function

$$a(t, \alpha) = \Re\left[K(\alpha + it) - K(\alpha)\right]. \tag{10}$$

Since $a(t, \alpha) = a(-t, \alpha)$ for $t \in \mathbb{R}$ and $a(0, \alpha) = 0$, straightforward algebra shows

$$\int_{-\infty}^{\infty} |g_x(t \pm id^\star)|dt = 2\frac{M(\bar{\bar{u}}_x \mp d^\star)}{M(\bar{\bar{u}}_x)} \int_0^{\infty} \frac{e^{a(t, \bar{\bar{u}}_x \mp d^\star)}}{\sqrt{(\bar{\bar{u}}_x \mp d^\star)^2 + t^2}} dt. \tag{11}$$

These integrals exist provided $e^{a(t,\alpha)} = O(t^{-\psi})$ for some $\psi > 0$ as $t \to \infty$. This condition is equivalent to requiring that the characteristic function of $X$ decay

to zero at least algebraically, and is thus satisfied provided the conditions of Theorem 2 hold.

Now, define

$$I_1(\alpha) = \int_{-L_\alpha}^{U} \frac{e^{a(e^s,\alpha)+s}}{\sqrt{\alpha^2+e^{2s}}} ds \quad \text{and} \quad I_2(\alpha) = \int_0^{1/U} \frac{e^{a(e^{1/s},\alpha)-1/s}}{s^2\sqrt{\alpha^2+e^{2/s}}} ds,$$

where $U > 0$ is arbitrary and

$$L_\alpha = \max\left[0, \frac{1}{2}\log\left(\frac{1-\tanh^2(\gamma)}{\alpha^2\tanh^2(\gamma)}\right)\right] \tag{12}$$

for $0 < \gamma < 1$. The following approximation result is proved in the Appendix.

**Proposition 1.** *Let* $0 < \gamma < 1$, $I(\alpha) = 2\,[M(\alpha)/M(\bar{\bar{u}}_x)] \times [I_1(\alpha) + I_2(\alpha)]$, *and*

$$\widehat{\mathcal{N}}_x = e^{-xd^\star} I(\bar{\bar{u}}_x + d^\star) + e^{xd^\star} I(\bar{\bar{u}}_x - d^\star). \tag{13}$$

*Then* $|\widehat{\mathcal{N}}_x - \mathcal{N}(g_x, D_{d^\star})| = O(2\gamma)$.

The integrals $I_1(\alpha)$ and $I_2(\alpha)$ involve finite limits of integration. More importantly, they involve integrands that decay exponentially, and thus (13) may be easily approximated using crude methods of numerical quadrature. In the examples of Section 5, $L_\alpha$ is computed as in (12) with $\gamma = 0.01$. Then, with $U = 10$, the integrals $I_1(\bar{\bar{u}}_x + d^\star)$ and $I_1(\bar{\bar{u}}_x - d^\star)$ are each computed with a simple Clenshaw-Curtis-type quadrature rule; see, for example, Krommer and Ueberhuber ((1998), §5.2.6) or Press et al. (1989, §5.7). The selection $U = 10$ is made both to ensure that $I_1(\bar{\bar{u}}_x \pm d^\star)$ is the dominant contribution to $I(\alpha)$ and to fix the computation of $I_2(\bar{\bar{u}}_x \pm d^\star)$ over a relatively small interval. The integrals $I_2(\bar{\bar{u}}_x + d^\star)$ and $I_2(\bar{\bar{u}}_x - d^\star)$ are each computed with a three-point Simpson rule, requiring a total of four additional function evaluations since $\lim_{s\to 0} s^{-2} e^{a(e^{1/s}, \bar{\bar{u}}_x \pm d^\star)} = 0$.

### 4.3. Bounding the appropriate choice of $h$

Define $\Delta_{min} = \max\{\log 2/(2d^\star), |x|\}$. Then, proceeding as in Theorem 2, $\Delta$ should be taken as the larger of $\Delta_{min}$ and the solution to $\mathcal{N}_x(g_x, D_{d^\star})\exp\{-2\Delta d^\star\} < \pi\epsilon_a e^{-\nu(\bar{\bar{u}}_x)}$. Substituting (13) in place of $\mathcal{N}_x(g_x, D_{d^\star})$, one finds that selecting

$$\Delta > \max\left(\Delta_{min}, \frac{1}{2d^\star}\log\left(\frac{e^{\nu(\bar{\bar{u}}_x)}\widehat{\mathcal{N}}_x}{\pi\epsilon_a}\right)\right) \tag{14}$$

ensures that the approximation error is either close to or bounded above by $\epsilon_a$. Since $h = \pi/\Delta$, selecting $\Delta$ in this way places an upper bound on $h$. A specific

choice of $\Delta$, hence $h$, satisfying the required inequalities is proposed in Section 4.5.1.

### 4.4. Handling truncation error

The main task is to compute (9) to within $\pm\epsilon_t$ of its actual value. For an integer $N \geq 2$, straightforward calculations yield

$$\frac{h}{2}\sum_{k=-\infty}^{\infty} g_x(kh)e^{-ixkh} = h\Big[g_x(0) + \sum_{k=1}^{N-1} R_x(kh)\Big] + E_N(h), \tag{15}$$

where $E_N(h) = h\sum_{k=N}^{\infty} R_x(kh)$ and $R_x(kh)$ is the real part of $g_x(kh)e^{-ixkh}$. Computing (15) to a guaranteed level of accuracy requires an upper bound on $|E_N(h)|$. Some limited insight here can be gained by rewriting $R_x(t)$ in a different form. Specifically let $a_x(t) = a(t, \bar{\bar{u}}_x)$, the latter being defined as in (10), and set $b_x(t) = \Im(K(\bar{\bar{u}}_x + it))$ to be its corresponding imaginary part. Then, it is easy to show that

$$R_x(t) = \frac{e^{a_x(t)}}{\bar{\bar{u}}_x^2 + t^2}\Big[\bar{\bar{u}}_x \cos(b_x(t) - xt) + t\sin(b_x(t) - xt)\Big] \tag{16}$$

and, consequently, that $|R_x(t)| \leq e^{a_x(t)}(\bar{\bar{u}}_x^2 + t^2)^{-1/2}$. This bound is typically monotone decreasing for $t > 0$, in which case

$$|E_N(h)| \leq \int_{(N-1)h}^{\infty} \frac{e^{a_x(t)}}{\sqrt{\bar{\bar{u}}_x^2 + t^2}}dt \tag{17}$$

(e.g., Abate and Whitt (1992, p.36)). The error bound (17) is usually very conservative. The conservatism occurs because the cancellation arising from oscillations in $R_x(t)$ about zero, captured by the bracketed term on the right hand side of (16), is ignored. Abate and Whitt (1992, 1995) show that conservative bounds like (17) can be avoided by instead exploiting oscillatory behavior in the terms of the series (15). The approach to be taken here will involve fixing $N$ to ensure that the terms in the tail series $E_N(h)$, properly grouped, exhibit approximately alternating behavior. The series $E_N(h)$ is then summed using a convergence acceleration method. Importantly, the substantial computational gains that can be achieved by doing so come at the expense of guaranteed accuracy.

The effective summation of (15) requires information on the pattern of oscillation in $R_x(t)$. Toward this end, first write $b_x(t) = \arg\left(\xi_R(t) + i\xi_I(t)\right)$, where $\xi_R(t)$ and $\xi_I(t)$ respectively denote the real and imaginary parts of $M(\bar{\bar{u}}_x + it)$ and $\arg z$ denotes the unique angle in $(-\pi, \pi]$ such that $z = |z|e^{i\arg(z)}$. For $z = x + iy$,

$\arg(z) = \text{sign}(y)\left\{\mathcal{H}(-x)\pi + [2\mathcal{H}(x) - 1]\arctan\left(|y/x|\right)\right\}$, where $\mathcal{H}(w)$ is defined as in (1). Consequently,

$$b_x(t) = \text{sign}(\xi_I(t))\left\{\mathcal{H}(-\xi_R(t))\pi + [2\mathcal{H}(\xi_R(t)) - 1]\arctan\left(\left|\frac{\xi_I(t)}{\xi_R(t)}\right|\right)\right\}. \quad (18)$$

The following result characterizes the behavior of $b_x(t)$ as $t \to \infty$ assuming certain conditions hold, and is important for developing insight into the behavior of $R_x(t)$.

**Proposition 2.** *Let the even and odd parts of $\varpi_T(s) = e^{\bar{\bar{u}}_x s}F'(s)$ be $\varpi_e(s) = (1/2)(\varpi_T(s) + \varpi_T(-s))$ and $\varpi_o(s) = (1/2)(\varpi_T(s) - \varpi_T(-s))$. As $s \downarrow 0$, suppose*

$$\varpi_e(s) \sim \frac{1}{2}\sum_{j=0}^{\infty}\gamma_{e,j}\ s^{j+\alpha_e-1} \quad \text{and} \quad \varpi_o(s) \sim \frac{1}{2}\sum_{j=0}^{\infty}\gamma_{o,j}\ s^{j+\alpha_o-1},$$

*where $\alpha_k > 0$, $k = e, o$. Then, under further smoothness and integrability conditions on $\varpi_k(\cdot)$ and its derivatives, $b_x(t) \to \theta$ as $t \to \infty$, where $\theta \in (-\pi, \pi]$ is a constant.*

The appearance of $\varpi_k(\cdot)$, $k = e, o$ in Proposition 2 stems from the dependence of $\xi_R(t)$ on $\varpi_e(\cdot)$ and $\xi_I(t)$ on $\varpi_o(\cdot)$. Implied in the expansions for $\varpi_k(s)$ as $s \downarrow 0$ is the assumption of either boundedness or unbounded integrability. For example, $\varpi_e(s)$ is bounded near $s = 0$ if $\alpha_e = 1$; $\varpi_o(s)$ is unbounded but integrable near $s = 0$ if $\alpha_o = 1/2$. Under these and other conditions on $\varpi_e(\cdot)$ and $\varpi_o(\cdot)$, $\xi_R(t)$ and $\xi_I(t)$ admit asymptotic expansions as $t \to \infty$ that are useful in studying the asymptotic behavior of $b_x(t)$.

Precise regularity conditions under which the stated expansions hold may be found in Wong (1989, §4.2)). Presently, the following loose interpretation is sufficient: if $\xi_I(t)$ and $\xi_R(t)$ are eventually of constant sign and their ratio tends to a unique (possibly infinite) limit as $t \to \infty$, then $b_x(t)$ tends to a unique limit $\theta \in (-\pi, \pi]$. Subsequent discussion regarding the oscillation patterns in $R_x(t)$ will be restricted to this case, and covers a large and useful class of interesting distributions. For example, if $\varpi_T(s)$ has nonnegative support (i.e., the random variable $X > 0$ with probability 1), then $\varpi_e(s) = \varpi_o(s) = (1/2)\varpi_T(s)$. Existence of the MGF of $X$ implies exponential decay of $F(x)$ and hence $F'(x)$ as $x \to \infty$. The existence of $\varpi_T(s) \sim \sum_{j=0}^{\infty}\gamma_j\ s^{j+\alpha-1}$ for some $\alpha > 0$ as $s \downarrow 0$ is then sufficient because the remaining regularity conditions can be shown to hold (cf. Wong (1989, §IV.2, Theorem 1)).

Assuming $b_x(t) \to \theta$ as $t \to \infty$, (16) implies that the cases $x = 0$ and $x \neq 0$ should be considered separately. Specifically, with $x = 0$, the oscillation in $R_x(t)$ dies out as $t \to \infty$; efficient computation of (15) then relies primarily on the decay rate of $t^{-1}e^{a_x(t)}$, and any reasonable quadrature rule can be employed. However,

if $x \neq 0$, the oscillation in $R_x(t)$ does not die out as $t \to \infty$. Computation of (15) then becomes more difficult, and it is helpful to obtain further insight into the zero patterns of $R_x(t)$. For $t > 0$ and integers $k$, the zeros of (16) arise as solutions to

$$b_x(t) - xt + k\pi = \arctan\left(-\frac{\bar{\bar{u}}_x}{t}\right). \tag{19}$$

Suppose $b_x(t) - xt \sim \theta - xt$ as $t \to \infty$, where $\theta \in (-\pi, \pi]$. Because $\arctan(-\bar{\bar{u}}_x\, t^{-1}) \sim -\bar{\bar{u}}_x t^{-1}$ as $t \to \infty$, the solutions of (19) are approximately given by the solutions to $\theta - xt + k\pi + \bar{\bar{u}}_x t^{-1} = 0$ or, equivalently, by $\hat{t}_k = \bar{\theta}_k + (2|x|)^{-1}\sqrt{\bar{\theta}_k^2 + 4x\bar{\bar{u}}_x}$ for $\bar{\theta}_k = \theta + k\pi$ and integers $k$ such that $\hat{t}_k$ is real and positive. It is expected that $\hat{t}_k$ will provide an accurate approximation for $t$ such that $b_x(t)$ is roughly constant and $t > 2|\bar{\bar{u}}_x|$; the latter condition arises because $|\arctan(u) - u| \leq 0.037$ for $|u| < 1/2$. Moreover, as $k \to \infty$,

$$\hat{t}_{k+1} - \hat{t}_k = \frac{\pi}{|x|} - \operatorname{sign}(x)\frac{\bar{\bar{u}}_x}{\pi k^2} + O(k^{-3}), \tag{20}$$

showing that the spacing between successive zeros settles down quickly.

This last observation is useful precisely because it implies $E_N(h)$, with its terms grouped properly, behaves like an alternating series for $N$ sufficiently large. Two "convergence acceleration" methods known to be effective for summing alternating series are Euler summation and the epsilon algorithm (e.g., see Brezinski and Redivo Zaglia (1991)); the latter is used in Section 4.5.2 below.

### 4.5. The main algorithm

The previous sections contain key details underlying the computational algorithm for

$$\widehat{P}\{X > x\} = \mathcal{H}(-\bar{\bar{u}}_x) + \frac{e^{\nu(\bar{\bar{u}}_x)}}{\pi}\Big[hg_x(0) + h\sum_{k=1}^{N-1} R_x(kh) + E_N(h)\Big], \tag{21}$$

where $R_x(\cdot)$ and $E_N(\cdot)$ are defined in Section 4.4. The main algorithm can now presented. Section 4.5.1 describes how $N$ and $h$ are determined; Section 4.5.2 describes how the epsilon algorithm is used in computing the "tail" of the infinite series (21), i.e., $\pi^{-1}e^{\nu(\bar{\bar{u}}_x)}E_N(h)$.

#### 4.5.1. Selection of $N$ and $h$

As discussed in Section 4.4, the initial truncation point $N$ is determined such that the terms in the series $E_N(h)$, when properly grouped, begin to exhibit regular alternating behavior. This is evidently connected to the behavior of $R_x(t)$ for $t \geq Nh$; consequently, the selection of $N$ and $h$ are linked as is described below:

1. Determine $z_0 > 0$ such that $R_x(z_0) = 0$ and the zeros of $R_x(t)$ for $t \geq z_0$ are approximately equally spaced. Specifically, the zeros $t_k$ of $R_x(t)$ for $t > 2|\bar{\bar{u}}_x|$ are successively computed until $t_{K+1}/t_K - 1 < 0.1$ for some $K \geq 1$, at which point $z_0 = t_K$.
2. As shown in (20), the predicted asymptotic spacing between successive zeros is $\varphi_0 = \pi/|x|$. If $|t_{K+1} - t_K - \varphi_0| < 0.1\varphi_0$, the spacing between successive zeros is set to $\varphi = \varphi_0$. However, if $t_{K+1}/t_K - 1 < 0.1$ and $|t_{K+1} - t_K - \varphi_0| \geq 0.1\varphi_0$, this indicates (20) may be incorrect. In this case, the spacing $\varphi$ is empirically determined, being set to the distance between $z_0$ and the next largest root of $R_x(t)$.
3. Compute $e_0 = z_0 + (\varphi/2)$, the first (approximate) extrema subsequent to $z_0$.
4. Set $N = \lfloor e_0\Delta_0/\pi \rfloor + 1$, $\Delta_N = N\pi/e_0$, and $h = \pi/\Delta_N$, where

$$\Delta_0 = \max\Big(\Delta_{min}, \frac{1}{2d^\star}\log\Big(\frac{e^{\nu(\bar{\bar{u}}_x)}\widehat{\mathcal{N}}_x}{\pi\epsilon_a}\Big)\Big).$$

Steps 1 and 2 can be computationally demanding. They can also be avoided if the user specifies $z_0$ and $\varphi$, computations typically requiring asymptotic analysis. Step 4 ensures $Nh = e_0$ and that $\Delta_N$ satisfies (14). If the zeros of $R_x(t)$ are approximately equally spaced for $t > e_0$, then the terms in $E_N(h)$ can be grouped to produce an approximately alternating series. The rationale for selecting $N$ such that $Nh$ coincides with an extrema (i.e., $e_0$) instead of a zero (i.e., $z_0$) is based on recommendations made in Sauter (2000). With these choices, an initial approximation $P_\star$ to (21) is:

$$P_\star = \mathcal{H}(-\bar{\bar{u}}_x) + \frac{e^{\nu(\bar{\bar{u}}_x)}}{\Delta_N}\Big[\frac{1}{\bar{\bar{u}}_x} + \sum_{k=1}^{N-1} R_x\Big(\frac{\pi k}{\Delta_N}\Big)\Big]. \tag{22}$$

### 4.5.2. Computing $\widehat{P}\{X > x\}$

The computation of (21) requires both $P_\star$ and $E_N(\pi/\Delta_N)$; the former is easily computed via (22), so the latter is now considered. Let $\alpha$ denote the nearest integer to $\varphi/h$. Then $E_N(\pi/\Delta_N) = [\pi/\Delta_N]\sum_{j=0}^{\infty}\beta_j$, with

$$\beta_j = \sum_{k=N+j\alpha}^{N+(j+1)\alpha-1} R_x\Big(\frac{k\pi}{\Delta_N}\Big). \tag{23}$$

Because $Nh = e_0$ is a point of extrema and $\alpha h$ approximates the period of $R_x(t)$, each $\beta_j$ is essentially a trapezoidal rule approximation to the integral of $R_x(t)$ between successive extrema. Provided $|g_x(t)e^{-ixt}|$ decays monotonically and the zeros of $R_x(t)$ are approximately equi-spaced for $t > Nh$, the $\beta_j'$s should be small in magnitude and alternate in sign.

Now, for $L \geq 0$, define the sequence $P_L = P_\star + (e^{\nu(\bar{\bar{u}}_x)}/\Delta_N)\sum_{j=0}^{L}\beta_j$. Notice that $P_\infty$ equals (21) for a specific choice of $h$ and $N$. Moreover, $P_L$ is just a linear transformation of $\sum_{j=0}^{L}\beta_j$ and corresponds to a partial sum of the desired infinite series. Hence the sequence of partial sums $\{P_L, L \geq 0\}$ should oscillate about the desired limit $P_\infty$. If so, the rate at which $P_L$ converges to $P_\infty$ can potentially be accelerated. The epsilon algorithm has been found to be effective when applied to sequences whose terms oscillate about a finite limit; see, for example, Smith and Ford (1982) and more recently Sauter (2000). Readers unfamiliar with this algorithm may wish to consult Wimp (1981), Brezinski and Redivo Zaglia (1991), or Sauter (2000).

Let $\varepsilon_L$ denote the result of applying the epsilon algorithm to a given sequence $\{P_0 \ldots P_L\}$, where $L \geq 0$. The exclusion of $P_\star$ as a member of this sequence is deliberate; the intent here is to accelerate the computation of the *tail* series $E_N(\pi/\Delta_N)$, or equivalently, $P_\infty - P_\star$. The computations for (21) are then finished adaptively as described below.

1. Set $L = 0$, compute $\varepsilon_0 = P_0$ and initialize $\mathsf{error}_{old}$ to be a large number.
2. Increment $L$ by 2, compute $P_{L-1}$ and $P_L$.
3. Compute $\varepsilon_L$ and $\mathsf{error}_{new} = |\varepsilon_L - \varepsilon_{L-2}|/\varepsilon_L$.
4. If $(1/3)\mathsf{error}_{old} + (2/3)\mathsf{error}_{new} < \epsilon_t/1000$, take $\varepsilon_L$ as the approximation and stop iteration; otherwise, set $\mathsf{error}_{old} = \mathsf{error}_{new}$ and return to step 2.

The reason for increasing the sequence length by two each time is connected to the difference in behavior of the epsilon algorithm when applied to sequences of even versus odd length; see, for example, Wimp (1981, p.141)) or Sauter (2000). The stopping criterion for checking convergence of the computed answer uses relative error and is set significantly smaller than the requested accuracy $\epsilon_t = (1/2)\epsilon_{tot}$. This is to help ensure that the final approximation matches the desired answer to (at least) the specified level of accuracy. The use of an unequally weighted average of the relative error across two successive iterations is used to guard against being fooled by locally small changes in the computed answer. The most recent iteration receives a larger weight since it is based on more quadrature points.

## 5. Examples

The examples below represent a subset of examples chosen to illustrate the performance of the proposed method across a reasonably diverse spectrum of problems; see Strawderman (2002) for several other examples. They were also chosen because it was possible to either compute or at least accurately approximate the tail probabilities using other methods, hence providing a basis for comparison. The computations were carried out in MAPLE 6 with floating point

precision set at 20 digits (i.e., Digits:=20; Waterloo Maple Inc., 2000). A copy of the MAPLE code used for these examples is available upon request.

All computations are carried out using $\epsilon_{tot} = 10^{-8}$. In addition to the CGF $K(t) = \log M(t)$, the only user input required is the ordinate $x$ and the set $\mathcal{E}$ for which $M(t)$, $t \in \mathcal{E}$ is finite. The computation of $\bar{u}_x$ requires $K'(\cdot)$; numerical differentiation is used here. In the tables, the absolute error of the approximations are reported. Also summarized are the values of $h$, $d^\star$, $\widehat{\mathcal{N}}_x$, and the number of points at which the CGF $K(\cdot)$ has been evaluated. This reported number of function evaluations reflects the computations involved in obtaining $\widehat{\mathcal{N}}_x$; and the quadrature nodes computed in Sections 4.5.1 and 4.5.2. However, it does not reflect those computations needed for determining $\bar{u}_x$, $z_0$ and $\varphi$ (see Sections 2.2 and 4.5.1). These computations rely on a built-in root finding subroutine, and the author was unable to obtain this information from MAPLE. However, as noted earlier, the numerical computation of $z_0$ and $\psi$ may also be viewed as optional since it absolves the user from doing the requisite asymptotic analysis. Consequently the reported number of function evaluations may be viewed as a measure of the efficiency of $\varepsilon_L$, given $z_0$, $\psi$ and $\bar{u}_x$.

For comparison, also reported are the absolute errors of the "straight trapezoidal rule" (i.e., unaccelerated) approximation $P_L$ and

$$\mathsf{Euler}(x) = P_\star + \frac{e^{\nu(\bar{u}_x)}}{\Delta_N 2^{L+1}} \sum_{k=0}^{L+1} \binom{L+1}{k} \Big[ \sum_{j=0}^{k} \beta_j \Big] \;\equiv\; P_\star + \frac{e^{\nu(\bar{u}_x)}}{\Delta_N} \sum_{j=0}^{L+1} w_j \beta_j,$$

where $w_j = P\{W \geq j\}$ for $W \sim \mathsf{Binomial}(L+1, 1/2)$. The approximation $\mathsf{Euler}(x)$ is obtained by adding the (truncated) Euler sum of the series $\sum_{j=0}^{\infty} \beta_j$ to the initial approximation $P_\star$. Euler summation is expected to be effective since $\beta_j$ and $\beta_{j+1}$ should have opposite signs and be decreasing in magnitude. Abate and Whitt (1992) provide a useful discussion on the application of Euler summation in similar problems. In the tables, the approximations $\varepsilon_L$ and $P_L$ are respectively referred to as $\mathsf{Epsilon}(x)$ and $\mathsf{Straight}(x)$. Importantly, each of these approximations is ultimately based on the same set of quadrature nodes, providing a balanced assessment of both accuracy and the effect of convergence acceleration. Finally, since one motivation of this paper is to provide a trustworthy alternative to saddlepoint methods, the absolute error of the Lugannani-Rice approximation

$$\mathsf{LR}(x) = 1 - \Phi(\hat{\omega}_x) + \phi(\hat{\omega}_x) \left[ \hat{z}_x^{-1} - \hat{\omega}_x^{-1} \right]$$

to $P\{X > x\}$ is also provided. Here, $\hat{z}_x = \mathrm{sign}(\hat{u}_x)\sqrt{K''(\hat{u}_x)}$, $\hat{\omega}_x = \mathrm{sign}(\hat{u}_x)$ $\sqrt{2[x\hat{u}_x - K(\hat{u}_x)]}$, and $K'(\hat{u}_x) = x$; see, for example, Kolassa (1997, Chap. 5). To a large extent, the tabulated results speak for themselves; comment is therefore reserved until Section 5.3, where some general observations are made.

### 5.1. Mixtures of independent non-central $\chi^2$ random variables

Let $\chi^2_p(\omega^2)$ denote a chi-squared random variable with $p$ degrees of freedom and noncentrality parameter $\omega^2$. The problems considered in this section deal with the mixture $X = \sum_{j=1}^n \lambda_j Y_j$, where $Y_j \sim \chi^2_{p_j}(\omega_j^2)$, $Y_j \perp Y_k$ for all $j \neq k$, $p_j > 0$ are integers, $\omega_j^2 \geq 0$, and $\lambda_j \in \mathbb{R}$ is nonzero. The MGF of $X$ takes the form $M_X(t) = \prod_{j=1}^n G(\lambda_j t; p_j, \omega_j^2)$ where $G(u; \nu, \eta^2) = (1-2u)^{-\nu/2} \exp\{\eta^2 u(1-2u)^{-1}\}$; see, for example, Johnson, Kotz and Balakrishnan (1995, Chap. 29). Importantly, the set $\mathcal{E}$ on which $M_X(t) < \infty$ is governed by the sign and magnitude of $\lambda_1 \ldots \lambda_n$. Davies (1980) notes that any quadratic form (or ratio thereof) in independent normal random variables can be reduced to the form $X + \sigma_0 Z$, where $Z \sim N(0,1)$, $Z \perp X$, and $\sigma_0 \geq 0$. Marsh (1998) obtains saddlepoint approximations for the ratio of quadratic forms in normal random variables, and demonstrates that the error of approximation decreases as $O(n^{-1})$. The numerical methods of this paper apply directly to this significant class of problems in statistics. Various methods of numerical inversion of the characteristic function for this problem have been considered previously; see, for example, Imhof (1961), Davies (1973, 1980), Rice (1980) and Helstrom (1983).

#### 5.1.1. An unweighted mixture

Consider $X = Y_1 + Y_2$, where $Y_1 \sim \chi^2_2(0.1)$ and $Y_2 \sim \chi^2_5(0.9)$. In this case, $X \sim \chi^2_7(1)$, and

$$P\{X > x\} = \frac{e^{-1/2}}{2^{7/2}\Gamma(7/2)} \int_x^\infty \left(s^{7/2} - 1\right) e^{-s/2} {}_0F_1\left(\frac{7}{2}, \frac{7s}{4}\right) ds,$$

with ${}_0F_1$ denoting a generalized hypergeometric series. The mean and standard deviation of $X$ are respectively 8 and 4.14. For the purposes of determining the approximation error of the various quadrature rules, the "exact" CDF is computed using MAPLE's built-in numerical integration routine to a requested accuracy of 20 digits. The results are reported in Table 1.

Table 1. Unweighted mixture of 2 noncentral chi-square random variables.

| | | | | # of | Absolute Error | | | |
|---|---|---|---|---|---|---|---|---|
| $x$ | $h$ | $d^\star$ | $\widehat{\mathcal{N}}_x$ | points | Straight$(x)$ | Epsilon$(x)$ | Euler$(x)$ | LR$(x)$ |
| 0.1 | 16.785 | 22.334 | 4.92 | 56 | $1.9 \times 10^{-11}$ | $1.6 \times 10^{-11}$ | $9.8 \times 10^{-12}$ | $1.7 \times 10^{-8}$ |
| 1.0 | 0.839 | 2.087 | 5.02 | 101 | $1.5 \times 10^{-8}$ | $1.7 \times 10^{-14}$ | $2.5 \times 10^{-9}$ | $1.3 \times 10^{-5}$ |
| 3.0 | 0.201 | 0.595 | 5.04 | 157 | $1.2 \times 10^{-7}$ | $1.6 \times 10^{-16}$ | $8.9 \times 10^{-10}$ | $5.6 \times 10^{-5}$ |
| 5.0 | 0.097 | 0.305 | 5.38 | 161 | $1.1 \times 10^{-6}$ | $5.3 \times 10^{-14}$ | $1.3 \times 10^{-7}$ | $5.8 \times 10^{-5}$ |
| 7.0 | 0.058 | 0.187 | 5.96 | 200 | $5.1 \times 10^{-7}$ | $1.9 \times 10^{-15}$ | $5.0 \times 10^{-8}$ | $2.1 \times 10^{-4}$ |
| 9.0 | 0.030 | 0.097 | 4.33 | 229 | $9.0 \times 10^{-8}$ | $2.2 \times 10^{-15}$ | $1.2 \times 10^{-8}$ | $2.9 \times 10^{-4}$ |
| 11.0 | 0.035 | 0.109 | 4.16 | 168 | $1.4 \times 10^{-6}$ | $4.1 \times 10^{-15}$ | $8.6 \times 10^{-8}$ | $2.8 \times 10^{-4}$ |

### 5.1.2. A weighted mixture supported on $\mathbb{R}$

Davies (1980, Table 3) considers computing the CDF for $X = 7\chi^2_6(6) + 3\chi^2_2(2) - 7\chi^2_1(6) - 3\chi^2_1(2)$. The support of $X$ is $\mathbb{R}$; the mean and standard deviation are respectively 38 and 56.88. The results of applying the present method to this problem may be found in Table 2. In this case a tractable formula for the CDF of $X$ is not available. "Exact" answers are obtained using algorithm AS155 of Davies (1980), which is specifically designed for this class of problems. The original FORTRAN 77 implementation of AS155 was modified for use with a high precision FORTRAN 95 compiler; computations were then carried out to a requested accuracy of $10^{-18}$. A minimum of 8102 quadrature points was required for the ordinates of Table 2.

Table 2. Weighted mixture of 4 noncentral chi-square random variables.

| | | | | # of | Absolute Error | | | |
|---|---|---|---|---|---|---|---|---|
| $x$ | $h$ | $d^\star$ | $\widehat{\mathcal{N}}_x$ | points | Straight$(x)$ | Epsilon$(x)$ | Euler$(x)$ | LR$(x)$ |
| -80.0 | 0.006 | 0.016 | 5.87 | 156 | $7.1 \times 10^{-12}$ | $4.7 \times 10^{-12}$ | $8.1 \times 10^{-11}$ | $2.8 \times 10^{-4}$ |
| -40.0 | 0.005 | 0.014 | 4.25 | 275 | $3.5 \times 10^{-12}$ | $3.6 \times 10^{-16}$ | $1.8 \times 10^{-11}$ | $1.1 \times 10^{-3}$ |
| -10.0 | 0.004 | 0.012 | 4.02 | 706 | $3.4 \times 10^{-14}$ | $6.1 \times 10^{-16}$ | $3.4 \times 10^{-11}$ | $1.8 \times 10^{-3}$ |
| 10.0 | 0.003 | 0.010 | 4.17 | 875 | $9.4 \times 10^{-14}$ | $2.2 \times 10^{-16}$ | $1.1 \times 10^{-10}$ | $9.9 \times 10^{-4}$ |
| 40.0 | 0.003 | 0.008 | 4.58 | 432 | $4.3 \times 10^{-12}$ | $2.2 \times 10^{-16}$ | $1.1 \times 10^{-10}$ | $1.8 \times 10^{-3}$ |
| 80.0 | 0.004 | 0.011 | 4.04 | 211 | $4.2 \times 10^{-11}$ | $2.0 \times 10^{-16}$ | $8.7 \times 10^{-10}$ | $2.1 \times 10^{-3}$ |
| 120.0 | 0.004 | 0.013 | 4.29 | 142 | $2.8 \times 10^{-11}$ | $4.4 \times 10^{-16}$ | $4.3 \times 10^{-10}$ | $7.2 \times 10^{-4}$ |

### 5.2. Time dependent mean of regulated Brownian motion

For $t \geq 0$, define $B^*(t) = B(t) - t - \min_{s\in[0,t]}\{B(s) - s\}$, where $B(t)$ denotes standard Brownian motion. Then, $B^*(t)$ is regulated Brownian motion with drift $-1$ and diffusion coefficient 1, and is useful for modeling stochastic flow systems arising in queuing theory. Evidently $B^*(t) \geq 0$; moreover, for $t > 0$ (see Abate and Whitt (1987)),

$$E\left[B^*(t)|B^*(0) = 0\right] = \frac{1}{2} - (t+1)\left[1 - \Phi(t)\right] + \sqrt{t}\ \phi(t), \tag{24}$$

where $\Phi(\cdot)$ and $\phi(\cdot)$ denote, respectively, the standard normal CDF and density functions. The MGF corresponding to (24) is $M(t) = 2(1 + (1-2t)^{1/2})^{-1}$; the mean and standard deviation are respectively 1/2 and 0.87. The CDF (24) corresponds to that of a mixture of two exponential random variables (Abate and Whitt (1987, Theorem 1.7)). While the density function $F'(t) = O(t^{-1/2})$ as $t \downarrow 0$, Theorem 2 still applies since the decay condition (7) is met with $r = 1/2$. Abate and Whitt (1992) use this example to demonstrate the performance of transform

inversion methods in a case where the terms in (15) decay slowly to zero. Their results can be summarized as follows: a combination of summation with Euler acceleration is far more effective than attempting to sum (15) directly. The results of applying the proposed method to this problem are summarized in Table 3. Notably, $F'(t) \sim \sqrt{2/(\pi t^3)}\exp(-t/2)$ for large $t$ (Abate and Whitt (1987, Cor. 1.3.5)), indicating that $F$ behaves like an Inverse Gaussian distribution in the upper tail. Consequently, it is reasonable to expect that $\mathsf{LR}(x)$ may perform well, particularly for extreme $x$ (cf. Daniels (1987, Table 1(b)), Jensen (1995, Ex. 2.4.7)).

Table 3. Time dependent mean of regulated Brownian motion.

| | | | | # of | Absolute Error | | | |
|---|---|---|---|---|---|---|---|---|
| $x$ | $h$ | $d^\star$ | $\widehat{\mathcal{N}}_x$ | points | $\mathsf{Straight}(x)$ | $\mathsf{Epsilon}(x)$ | $\mathsf{Euler}(x)$ | $\mathsf{LR}(x)$ |
| 0.1 | 2.095 | 7.037 | 13.57 | 345 | $3.3 \times 10^{-4}$ | $1.5 \times 10^{-17}$ | $6.8 \times 10^{-8}$ | $3.4 \times 10^{-2}$ |
| 0.5 | 0.038 | 0.125 | 16.05 | 3313 | $1.3 \times 10^{-4}$ | $1.1 \times 10^{-16}$ | $4.3 \times 10^{-8}$ | — |
| 1.0 | 0.038 | 0.125 | 16.23 | 1591 | $1.1 \times 10^{-4}$ | $6.1 \times 10^{-16}$ | $2.0 \times 10^{-7}$ | $2.7 \times 10^{-2}$ |
| 2.0 | 0.038 | 0.125 | 16.80 | 888 | $1.4 \times 10^{-4}$ | $3.8 \times 10^{-17}$ | $2.6 \times 10^{-8}$ | $1.3 \times 10^{-2}$ |
| 4.0 | 0.039 | 0.125 | 18.73 | 454 | $4.6 \times 10^{-4}$ | $4.0 \times 10^{-17}$ | $2.2 \times 10^{-8}$ | $3.5 \times 10^{-3}$ |
| 6.0 | 0.039 | 0.125 | 21.85 | 309 | $3.9 \times 10^{-4}$ | $3.5 \times 10^{-17}$ | $1.7 \times 10^{-8}$ | $9.7 \times 10^{-4}$ |
| 8.0 | 0.040 | 0.125 | 26.33 | 275 | $1.9 \times 10^{-4}$ | $8.6 \times 10^{-18}$ | $2.8 \times 10^{-9}$ | $2.8 \times 10^{-4}$ |
| 10.0 | 0.041 | 0.125 | 32.47 | 227 | $1.0 \times 10^{-4}$ | $2.2 \times 10^{-17}$ | $2.3 \times 10^{-9}$ | $8.5 \times 10^{-5}$ |

### 5.3. Summary of results

In general, the tables here and in Strawderman (2002) show that $\mathsf{Epsilon}(x)$ significantly outperforms both $\mathsf{Straight}(x)$ and $\mathsf{Euler}(x)$ in terms of absolute accuracy. It is also evident that the epsilon algorithm substantially improves upon Euler summation as a method for accelerating the computation of the infinite series $P_\infty$. The greatest benefit of using the epsilon algorithm occurs in Table 3. In this case $R_x(t)$ decays slowly, and $\mathsf{Straight}(x)$ provides a comparatively poor approximation; in contrast, $\mathsf{Euler}(x)$ roughly doubles and $\mathsf{Epsilon}(x)$ roughly triples the number of correct significant digits. Tables 1 and 2 also display impressive gains. The following general trends are present:

- $h$, $d^\star$ and $\widehat{\mathcal{N}}_x$ can vary significantly with the ordinate $x$;
- the number of quadrature nodes required is typically greatest for ordinates $x$ close to $E[X]$, and decays in the tails;
- $\mathsf{Epsilon}(x)$ significantly exceeds the requested accuracy of $\epsilon_{tot} = 10^{-8}$ in all cases;
- $\mathsf{LR}(x)$ provides an erratic and comparatively inaccurate approximation to $P\{X > x\}$, though it often improves for extreme values of $x$.

## 6. Discussion

The trapezoidal rule is well known and has been proposed as a way to integrate the tail probability inversion integral in a number of previous papers. This paper is the first to apply the results of Stenger (1993) to this problem. Theorem 2 shows that the conditions required on the distribution of the random variable $X$ are fairly weak, the most restrictive being existence of the MGF. From the perspective of the literature on sinc quadrature rules (see e.g., Lund and Bowers (1992) or Stenger (1993)), a novel feature of this work is the attention paid to computing $\mathcal{N}_x(g_x, D_{d^\star})$. The proposal of Section 4.2 for approximating $\mathcal{N}_x(g_x, D_{d^\star})$ is new and facilitates choosing $h$ with confidence. As stated, Proposition 1 is restricted to the specific problem at hand. However, the essential assumptions on the integrand(s) are boundedness at the origin and algebraic decay, and thus the basic ideas apply more generally.

The examples here and in Strawderman (2002) demonstrate that proposed methodology works very well. The results support the conclusions of Abate and Whitt (1992) that numerical transform inversion can be done accurately and (relatively) easily. The current algorithm is an improvement over existing technology for univariate transform inversion in the sense that the same algorithm may be applied without regard to the support of the distribution of $X$. However, other choices exist, especially for the inversion of one-sided Laplace transforms; see Abate and Whitt (1992, §15) for a review. Most of these algorithms are also derived from the trapezoidal rule, but are otherwise distinct from the proposed method. The algorithm EULER of Abate and Whitt (1992, 1995) is one elegant example. EULER is surprisingly easy to code and could have been used in all cases except Section 5.1.2. However, the simplicity of EULER is due to its ignorance of certain considerations addressed in detail here. In particular, EULER requires specifying two parameters $n$ and $m$ whose roles are analogous to those of $N$ and $L$; the former determines at what point in the series acceleration is begun, the latter determines how many terms are used in actually approximating the "tail." Abate and Whitt (1995) remark that "we typically use $m = 11$ and $n = 15$, increasing $n$ as necessary." The selection $m = 11$ assumes that the tail series being summed is alternating. Because EULER employs $h = \pi/(2x)$, knowing whether or not this is the case is equivalent to the problem of determining $n$ such that the sign pattern of the integrand has indeed become "regular"; see Section 4.5.1. The EULER algorithm expends no effort to determine whether this is indeed the case.

The proposed methodology uses convergence acceleration to achieve the high levels of accuracy observed in the tables. Though the utility and effectiveness of convergence acceleration are apparent, these gains come at the expense of a rather complicated computational methodology. In practice, tail probabilities are rarely

needed to the level of accuracy reported in the tables. Indeed, $\mathsf{LR}(x)$ arguably provides an adequate answer in most cases, and is relatively easy to compute. However, Table 3 demonstrates that this is not always the case, despite the fact that the theory suggests it may have potential. This is perhaps symptomatic of saddlepoint methods: trustworthy guidelines for their successful application are not available, in part because sharp error bounds are either difficult or impossible to obtain. To a significant degree, then existing evidence of their accuracy in statistical applications is arguably anecdotal. In contrast, the theory of this paper provides a computable bound on the approximation error associated with (9). These results ensure that $P\{X > x\}$ can be computed to as many significant digits as desired simply by summing enough terms. For example, one may simply use $\mathsf{Straight}(x)$; that is, compute $h$ according to (14) and then simply increase $N$ in (21) until the answer stabilizes at the desired number of significant digits. This simple but somewhat inefficient method of approximation creates a rather happy medium: when more moderate levels of accuracy are desired (e.g., $10^{-4}$), the straight trapezoidal rule provides a simple computational method whose error is under complete user control.

The proposed methodology only requires specifying the cumulant (or moment) generating function of a univariate random variable. This covers a large number of interesting situations, including the computation of conditional distribution functions. For example, the algorithm described here may in principle be applied in problems for which Skovgaard's conditional tail probability approximation can be used (Skovgaard (1987)). However, in order to do so, the corresponding conditional cumulative generating function is needed, and this presents a significant drawback (cf. Kolassa (1997, §7.2)). Put another way, the computations required parallel those needed for a "single", rather than "double", saddlepoint approximation to the desired conditional probability. Successfully circumventing this problem might be accomplished by extending Theorem 1 to multivariate transforms; for related work in this direction, see Choudhury, Lucantoni, and Whitt (1994).

This paper has focused on the case in which $X$ is absolutely continuous. Computations for lattice-valued random variables are significantly easier because the inversion integral (1) can be expressed over a finite range (cf. Kolassa (1997, §2.7)). In this case the main challenge lies in obtaining a useful bound on the approximation error; the difficulties dealt with in Section 4.4 do not arise. A useful approach for handling lattice-valued random variables is described in Abate and Whitt (1992); another can be derived using Stenger's results. Computations presenting greater challenges for "Fourier series" methods include cases in which (i) $X$ has a density but not a MGF (e.g., Cauchy random variables); (ii) $X$ is discrete but not lattice-valued; and (iii), the CDF of $X$ is continuous but

not everywhere differentiable. The difficulties stem from slow decay rates of the Fourier transform and (at points of discontinuity) the Gibbs Phenomenon. Smoothing is likely to be required to successfully cope with such problems.

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## Appendix. Proofs

**Proof of Theorem 2.**

For $h = \pi/\Delta$, the conditions on $\Delta$ become equivalent to the stated conditions on $h$ in Theorem 1. Also, from (4), observe that

$$\begin{aligned}&\Big|P\{X > x\} - \Big[\mathcal{H}(-\bar{u}_x) + \frac{e^{\nu(\bar{u}_x)}}{\pi}\mathcal{I}_x(h)\Big]\Big| \\ &= \frac{e^{\nu(\bar{u}_x)}}{2\pi}\Big|\int_{-\infty}^{\infty} g_x(t)e^{-ixt}dt - \sum_{k=-\infty}^{\infty} g_x(kh)e^{-ixkh}\Big|.\end{aligned}$$

Hence, the result follows directly from Theorem 1 provided (i)-(iii) are satisfied under the stated conditions.

Let $z = s + iy \in \mathbb{C}$, and let $D_a \subset \mathbb{C}$ denote the infinite strip of width $a > 0$ containing the real axis. We must first establish (i)-(iii) of Theorem 1 for $f = g_x$. To show (i), recall first that $g_x(z) = \exp\{K(\bar{u}_x - y + is) - K(\bar{u}_x)\}/(\bar{u}_x - y + is)$. Using known results on the analyticity of the composition of two analytic functions and properties of $\exp\{K(iz)\}$ (e.g., Lukacs (1970, Chap. 7)), it follows that $g_x(z)$ is analytic in $D_{d^\star}$ provided $d^\star$ is strictly less than the upper bounds specified in (8).

Let $d^\star$ satisfy the stated conditions. Then, in order to prove (ii), it must be shown that

$$\int_{-d^\star}^{d^\star} |g_x(s + iy)|dy = \int_{-d^\star}^{d^\star} \frac{|\exp\{K(\bar{u}_x - y + is) - K(\bar{u}_x)\}|}{\sqrt{(\bar{u}_x - y)^2 + s^2}}dy \tag{25}$$

decays to zero as $|s| \to \infty$. Since $|y| \le d^\star$, it follows that $|K(\bar{u}_x - y)| < \infty$; moreover, $|\exp\{K(\bar{u}_x - y + is) - K(\bar{u}_x - y)\}| \le 1$ for all $s \in \mathbb{R}$. Consequently,

$$|\exp\{K(\bar{u}_x - y + is) - K(\bar{u}_x)\}| \le \exp\{K(\bar{u}_x - y) - K(\bar{u}_x)\} < \infty,$$

and the right-hand side of (25) goes to zero as $|s| \to \infty$.

To prove (iii), let $y \to (d^\star)^-$. Then, with $M(u) = \exp\{K(u)\}$ and $z = s \pm id^\star$,

$$|g_x(z)| = \frac{M(\bar{u}_x \mp d^\star)}{M(\bar{u}_x)} \times \frac{|\exp\{K(\bar{u}_x \mp d^\star + is) - K(\bar{u}_x \mp d^\star)\}|}{\sqrt{(\bar{u}_x \mp d^\star)^2 + s^2}}. \tag{26}$$

The restrictions on $d^\star$ ensure that $M(\bar{u}_x \mp d^\star) < \infty$ and $(\bar{u}_x \mp d^\star)^2 > 0$. This, combined with the ridge property of characteristic functions (e.g., Lukacs (1970)), implies the integrand is bounded and exists for $s = 0$. Provided $|\exp\{K(\bar{u}_x \mp d^\star + is) - K(\bar{u}_x \mp d^\star)\}| = O(|s|^{-r})$ as $|s| \to 0$ for some $r > 0$, (26) is $o(|s|^{-1})$ as $|s| \to \infty$ and therefore integrable.

Let $F'(\cdot)$ denote the probability density function associated with the CDF $F(\cdot)$ of $X$; note that $F'(\cdot)$ exists since $X$ is assumed to be absolutely continuous. Then,

$$\exp\{K(\bar{u}_x \mp d^\star + is) - K(\bar{u}_x \mp d^\star)\} = \int_{-\infty}^{\infty} e^{isu} \left[ \frac{e^{(\bar{u}_x \mp d^\star)u} F'(u)}{M(\bar{u}_x \mp d^\star)} \right] du.$$

The right-hand side is exactly the same as the left-hand side of (7) with $\beta = \bar{u}_x \mp d^\star$ and thus satisfies the needed condition. Since $M(\bar{u}_x \mp d^\star) < \infty$ by construction, (26) and arguments just given now establish the requisite boundedness, completing the proof.

**Proof of Proposition 1.** The function $\exp\{a(t, \bar{\bar{u}}_x \mp d^\star)\}$ may decay slowly (i.e., algebraically) to zero as $t \to \infty$, making the integral on the right-hand side of (11) more challenging to compute. This difficulty is alleviated by making the change of variable $t = e^s$:

$$\int_0^\infty \frac{e^{a(t, \bar{\bar{u}}_x \mp d^\star)}}{\sqrt{(\bar{\bar{u}}_x \mp d^\star)^2 + t^2}} dt = \int_{-\infty}^\infty e^{a(e^s, \bar{\bar{u}}_x \mp d^\star)} \frac{e^s}{\sqrt{(\bar{\bar{u}}_x \mp d^\star)^2 + e^{2s}}} ds. \tag{27}$$

To see why, let $\alpha$ equal one of $\bar{\bar{u}}_x \pm d^\star$, and note that $\alpha \neq 0$ by the choice of $d^\star$. Then, since $0 < e^{a(e^s, \alpha)} \leq 1$ for $s \in \mathbb{R}$, the integrand on the right-hand side of (27) is $O(e^{-|s|})$ as $s \to -\infty$. In addition, since $e^{a(t,\alpha)} = O(t^{-\psi})$ as $t \to \infty$, the integrand on the right-hand side of (27) is $O(e^{-\psi s})$ as $s \to \infty$. Consequently the tails of the integrand on the right-hand side of (27) vanish exponentially, making it easier to integrate numerically.

In computing (27), the lower and upper tails of the integrand are handled differently. This is because successful truncation of the upper tail requires additional information about the decay rate of $e^{a(t,\alpha)}$ as $t \to \infty$. With $\alpha = \bar{\bar{u}}_x \pm d^\star$, (27) may be written as

$$\int_{-\infty}^{-L_\alpha} \frac{e^{a(e^s, \alpha) + s}}{\sqrt{\alpha^2 + e^{2s}}} ds + I_1(\alpha) + I_2(\alpha), \tag{28}$$

the presence of $I_2(\alpha)$ following from the fact that

$$\int_U^\infty \frac{e^{a(e^s, \alpha) + s}}{\sqrt{\alpha^2 + e^{2s}}} ds \equiv \int_0^{1/U} \frac{e^{a(e^{1/s}, \alpha) - 1/s}}{s^2 \sqrt{\alpha^2 + e^{2/s}}} ds$$

for $U > 0$. Now, note that

$$\int_{-\infty}^{-L} e^{a(e^s,\alpha)} \frac{e^s}{\sqrt{\alpha^2 + e^{2s}}} ds \leq \int_L^{\infty} \frac{e^{-s}}{\sqrt{\alpha^2 + e^{-2s}}} ds = \tanh^{-1}\left(\frac{1}{\sqrt{\alpha^2 e^{2L} + 1}}\right)$$

for $L > 0$. Hence, taking $L$ equal to (12), the first term in (28) is bounded above by $\gamma$ and thus $I_1(\alpha) + I_2(\alpha)$ approximates (27) to within $\gamma$. The result now follows by noting that $\mathcal{N}(g_x, D_{d^\star})$ is simply a weighted sum of two such terms.

**Proof of Proposition 2.** Because $M(\bar{\bar{u}}_x + it)$ is the Fourier transform of $\varpi_T(s) = e^{\bar{\bar{u}}_x s} F'(s)$,

$$M(\bar{\bar{u}}_x + it) = \int_{-\infty}^{\infty} e^{its} \varpi_T(s) ds = 2\int_0^{\infty} \cos(ts)\varpi_e(s) ds + 2i \int_0^{\infty} \sin(ts)\varpi_o(s) ds,$$

the second line implying that $\xi_R(t) = 2\int_0^{\infty} \cos(ts)\varpi_e(s) ds$ and $\xi_I(t) = 2\int_0^{\infty} \sin(ts)\varpi_o(s) ds$.

Consider first $\xi_R(t) = 2\int_0^{\infty} \cos(ts)\varpi_e(s) ds = 2\Re\{\int_0^{\infty} e^{its}\varpi_e(s) ds\}$. By results in Wong (1989, §IV.2), the asymptotic expansion for $\varpi_e(s)$ as $s \downarrow 0$ implies

$$\xi_R(t) \sim \frac{\gamma_{e,0} \cos\left(\frac{\pi\alpha_e}{2}\right) \Gamma(\alpha_e)}{t^{\alpha_e}} + \frac{\gamma_{e,1} \cos\left(\frac{\pi(\alpha_e+1)}{2}\right) \Gamma(\alpha_e + 1)}{t^{\alpha_e+1}} + o(t^{-(\alpha_e+1)}), \quad t \to \infty.$$

Similarly, as $t \to \infty$,

$$\xi_I(t) \sim \frac{\gamma_{o,0} \sin\left(\frac{\pi\alpha_o}{2}\right) \Gamma(\alpha_o)}{t^{\alpha_o}} + \frac{\gamma_{o,1} \sin\left(\frac{\pi(\alpha_o+1)}{2}\right) \Gamma(\alpha_o + 1)}{t^{\alpha_o+1}} + o(t^{-(\alpha_o+1)}).$$

Thus, $\xi_I(t)$ and $\xi_R(t)$ are of constant sign as $t \to \infty$. Moreover, it can be shown that

$$\frac{\xi_I(t)}{\xi_R(t)} \sim \begin{cases} \pm\infty & \alpha_e > \alpha_o > 0 \\ \dfrac{\gamma_{o,0}\sin(\frac{\pi\alpha}{2})\Gamma(\alpha) + \gamma_{o,1}\sin(\frac{\pi(\alpha+1)}{2})\Gamma(\alpha+1)t^{-1} + o(t^{-1})}{\gamma_{e,0}\cos(\frac{\pi\alpha}{2})\Gamma(\alpha) + \gamma_{e,1}\cos(\frac{\pi(\alpha+1)}{2})\Gamma(\alpha+1)t^{-1} + o(t^{-1})} & \alpha_e = \alpha_o = \alpha > 0 \\ 0 & 0 < \alpha_e < \alpha_o. \end{cases}$$

The limit in the case where $\alpha_e = \alpha_0$ depends on the structure of the expansions for $\varpi_e(s)$ and $\varpi_o(s)$, and in particular on the coefficient sequences $\gamma_{k,j}$, $j \geq 0$, $k = e, o$. In the present situation, the only important implication is that a unique limit exists, whether or not it is finite. These observations, combined with the fact that $\xi_I(t)$ and $\xi_R(t)$ become of constant sign as $t \to \infty$, now imply that

$$\arctan\left(\left|\frac{\xi_I(t)}{\xi_R(t)}\right|\right) \sim \begin{cases} \frac{\pi}{2} & \alpha_e > \alpha_o > 0 \\ \theta_0 & \alpha_e = \alpha_o = \alpha > 0 \\ 0 & 0 < \alpha_e < \alpha_o, \end{cases}$$

where $\theta_0 \in [-\pi/2, \pi/2]$. The stated result now follows from (18).

## References


Abate, J. and Whitt, W. (1987). Transient behavior of regulated Brownian motion I: starting at the origin. *Adv. Appl. Probab.* **19**, 560-598.

Abate, J. and Whitt, W. (1992). The Fourier series method for inverting transforms of probability distributions. *Queueing Systems* **10**, 5-87.

Abate, J. and Whitt, W. (1995). Numerical inversion of Laplace transforms of probability distributions. *ORSA J. Comput.* **7**, 36-43.

Abate, J., Choudhury, G. and Whitt, W. (1999). An introduction to numerical transform inversion and its application to probability models. In *Computational Probability* (Edited by W. Grassman). Kluwer, Boston.

Bak, J. and Newman, D. J. (1996). *Complex Analysis.* 2nd edition. Springer-Verlag, New York.

Barndorff-Nielsen, O. E. and Cox, D. R. (1989). *Asymptotic Techniques for Use in Statistics.* Chapman-Hall, London.

Barndorff-Nielsen, O. E. and Cox, D. R. (1994). *Inference and Asymptotics.* Chapman-Hall, London.

Bleistein, N. L. and Handelsman, R. A. (1975). *Asymptotic Expansions of Integrals.* Dover, New York.

Böhman, H. (1975). Numerical inversion of characteristic functions. *Scand. Actuar. J.* **2**, 121-124.

Brezinski, C. and Redivo Zaglia, M. (1991). *Extrapolation Methods: Theory and Practice.* North-Holland, Amsterdam.

Butzer, P. L. and Stens, R. L. (1983). The Poisson summation formula, Whittaker's cardinal series and approximate integration. In *Second Edmonton Conference on Approximation Theory*, Canadian Mathematical Society Conference Proceedings (Edited by Edmonton, Alberta, 1982). American Mathematical Society, Providence.

Choudhury, G. L., Lucantoni, D. M. and Whitt, W. (1994). Multidimensional transform inversion with applications to the transient $M/G/1$ queue. *Ann. Appl. Probab.* **4**, 719-740.

Daniels, H. (1954). Saddlepoint approximations in statistics. *Ann. Math. Statist.* **25**, 631-650.

Daniels, H. (1983). Saddlepoint approximations for estimating equations. *Biometrika* **70**, 89-96.

Daniels, H. (1987). Tail probability approximations. *Internat. Statist. Rev.* **55**, 37-48.

Davies, R. B. (1973). Numerical inversion of a characteristic function. *Biometrika* **60**, 415-417.

Davies, R. B. (1980). [Algorithm AS 155] The distribution of a linear combination of $\chi^2$ random variables. *Appl. Statist.* **29**, 323-333.

Davis, P. and Rabinowitz, P. (1984). *Methods of Numerical Integration.* 2nd edition. Academic Press, New York.

Davison, A. C. (1988). Approximate conditional inference in generalized linear models. *J. Roy. Statist. Soc. Ser. B* **50**, 445-461.

Feller, W. (1971). *An Introduction to Probability Theory and its Applications*, Vol. 2. 2nd edition. Wiley, New York.

Field, C. A. and Ronchetti, E. (1990). *Small Sample Asymptotics, IMS* Lecture Notes Vol. 13, Institute of Mathematical Statistics, Hayward.

Helstrom, C. W. (1983). Comment on "Distribution of quadratic forms in normal random variables−evaluation by numerical integration." *SIAM J. Sci. Statist. Comput.* **4**, 353-356.

Imhof, J. P. (1961). Computing the distribution of quadratic forms in normal variables. *Biometrika* **48**, 419-426.

Jensen, J. L. (1995). *Saddlepoint Approximations.* Clarendon Press, Oxford.

Johnson, N. L., Kotz, S. and Balakrishnan, N. (1995). *Continuous Univariate Distributions.* Vol. 2. 2nd edition. Wiley, New York.

Kawata, T. (1972). *Fourier Analysis in Probability Theory.* Academic Press, New York.

Kolassa, J. (1997). *Series Approximation Methods in Statistics.* 2nd edition. Springer-Verlag, New York.

Krommer, A. R. and Ueberhuber, C. W. (1998). *Computational Integration.* Society for Industrial and Applied Mathematics, Philadelphia.

Lugannani, R. and Rice, S. O. (1980). Saddlepoint approximation for the distribution of the sum of independent random variables. *Adv. Appl. Probab.* **12**, 475-490.

Lukacs, E. (1970). *Characteristic Functions.* 2nd edition. Griffin, London.

Lund, J. and Bowers K. L. (1992). *Sinc Methods for Quadrature and Differential Equations.* Society for Industrial and Applied Mathematics, Philadelphia.

Marsh, P. W. N. (1998). Saddlepoint approximations for noncentral quadratic forms. *Econom. Theory* **14**, 539-559.

Mehta, C. R., Senchaudhuri, P. and Patel, N. (1998). Discussion of "Approximately exact inference for the common odds ratio in several $2 \times 2$ tables" by Strawderman and Wells. *J. Amer. Statist. Assoc.* **93**, 1313-1316.

Olver, F. W. J. (1974). *Asymptotics and Special Functions.* Academic Press, New York.

Press, W. H., Flannery, B. P., Teukolsky, S. A. and Vetterling, W. T. (1989). *Numerical Recipes: The Art of Scientific Computing* (FORTRAN Version). Cambridge University Press, Cambridge.

Rice, S. O. (1980). Distribution of quadratic forms in normal random variables−evaluation by numerical integration. *SIAM J. Sci. Statist. Comput.* **1**, 438-448.

Sauter, T. (2000). Computation of irregularly oscillating integrals. *Appl. Numer. Math.* **35**, 245-264.

Skovgaard, I. M. (1987). Saddlepoint expansions for conditional distributions. *J. Appl. Probab.* **24**, 875-887.

Smith, D. A. and Ford, W. F. (1982). Numerical comparisons of nonlinear convergence accelerators. *Math. Comput.* **38**, 481-499.

Stenger, F. (1993). *Numerical Methods Based on Sinc and Analytic Functions.* Springer-Verlag, New York.

Strawderman, R. L. (2000). Higher-order asymptotic approximation: Laplace, saddlepoint, and related methods. *J. Amer. Statist. Assoc.* **95**, 1358-1364.

Strawderman, R. L. (2002). Computing tail probabilities by numerical Fourier inversion: the absolutely continuous case. Biometrics Technical Report BU-1605, Cornell University.

Titchmarsh, E. C. (1948). *Introduction to the Theory of Fourier Integrals.* 2nd edition. Clarendon Press, Oxford.

Waller, L. A., Turnbull, B. W. and Hardin, J. M. (1995). Obtaining distribution functions by numerical inversion of characteristic functions with applications. *Amer. Statist.* **49**, 346-350.

Waterloo Maple Inc. (2000). *Maple* 6 *for Linux.* Waterloo Maple Software, Waterloo.

Wimp, J. (1981). *Sequence Transformations and Their Applications.* Academic Press, New York.

Wong, R. (1989). *Asymptotic Approximations of Integrals.* Academic Press, Boston.

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