Closed Analytical Forms and Numerical Approximation of Dickey-Fuller Probability Distributions

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Abstract

A discrete real time series is often modelled by an autoregressive equation, the simplest kind of which is first order autoregression without deterministics:

$$X_t = \alpha X_{t-1} + \varepsilon_t, \quad t = 1, 2, ..., T,$$

with independent and $N(0, \sigma^2)$ distributed errors $\varepsilon_1, ..., \varepsilon_T$. Statistical inference about α can be drawn, for instance, by testing a null hypothesis of the form $H_0 : \alpha = \alpha_0$ for an $\alpha_0 \in R$ against some alternative. The present thesis is interested in testing the particularly important random walk hypothesis $H_0 : \alpha = 1$, and, more precisely, in the limiting (Dickey Fuller) distributions as $T \to \infty$ under H_0 of the two most common test statistics: the normalised coefficient estimator $T(\hat{\alpha}_T - 1)$ and the t ratio $(\hat{\alpha}_T - 1)/\hat{\sigma}_{\hat{\alpha}_T}$. The same limiting distributions also arise when testing for a unit root in a wide range of more general time series models. This thesis seeks to derive integral-free analytical expressions for these limiting distribution – a problem which has been open for decades and was for the first time tackled by K. Abadir (e.g. 1993, Ann. Statist. 21, p. 1058-70).

The thesis has both a mathematical aim (Chapter 2) and a numerical aim (Chapters 3 & 4). Chapter 2 derives new closed analytical expressions for the above-mentioned limiting distributions in the form of converging infinite series of elementary and special functions. Meanwhile some propositions of general interest on distributions on $\mathbf{R}^n$ are proved. Chapter 3 treats the question of the convergence rates of the occurring series and hence of their appropriate truncation. Based on these results, Chapter 4 discusses the numerical implementation and derives highly accurate tables of quantiles and other quantities.

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Chapter 1

Introduction

The aim of this introductory chapter is first to motivate the research undertaken by this thesis (cf. Section 1.1), then to give an overview of the main techniques and results (cf. Section 1.2), and finally to place our results into a broader statistical context (cf. Section 1.3). The time series model chosen in Section 1.1 is the simplest model in which the relevant asymptotic distributions of unit root tests arise, namely the Gaussian autoregressive order 1 ("AR(1)") model. In this model, testing for a unit root is equivalent to testing for a random walk, and the importance of such tests is easily described. The summary given in Section 1.2 contains a qualitative overview of the main mathematical and numerical results as well as a sketch of the techniques employed to reach these results. In the general statistical discussion of Section 1.3 we among others discuss the peculiarity of unit root (limiting) distributions in hypothesis testing; we further mention a wide class of more general time series models in which unit root testing gives rise to the asymptotic distributions studied here.

Some conventions and notation are introduced in Section 1.4.

1.1 Motivation

The motivation for unit root testing in one-dimensional time series and for the particular aims of this thesis is easiest described by considering the simple Gaussian AR(1) model. In this model, the unit root hypothesis is equivalent to the random walk hypothesis. It should however be pointed out that the discussion of this section could be translated to more general models, either with higher autoregression orders or with generalised error processes such as errors that are non-Gaussian with possibly heterogeneous and/or dependent distributions; these model extensions are discussed in Section 1.3.6.

The present section begins by introducing the relevant unit root test statistics (Sections 1.1.1 and 1.1.2); we then discuss the asymptotic (Dickey-Fuller) distribution of these test statistics and present some motivation for an analytical description of these distributions as undertaken by this thesis (cf. Sections 1.1.3 and 1.1.4).

1.1.1 The model and the random walk hypothesis

A classical way of modelling the probabilistic behaviour of a discrete real time series $(X_t)_{t=0,...,T}$ (for some sample size $T \in \{1, 2, ...\}$) is to explain X_t by its own past values. In the case that this dependence can be assumed linear, this leads to a linear autoregressive model. When the present value depends on past values only through the immediately past value, then the autoregressive order is 1. If, further, the time series contains no deterministic components such as a linear or seasonal trend, $(X_t)_{t=0,...,T}$ satisfies the AR(1) difference equation:

$$X_t = \alpha X_{t-1} + \eta_t, \quad t = 1, 2, ..., T. \tag{1.1}$$

We here assume that the error process $\eta_1, ..., \eta_T$ is a sequence of independent Gaussian variables $\eta_t \sim N(0, \sigma^2)$ with unknown variance $\sigma^2 > 0$. Further, the initial value X_0 is assumed to be fixed, i.e. the model is conditional on X_0. The process X_t can be expressed in terms of X_0 and $\eta_1, ..., \eta_t$, giving

$$X_t = \alpha^t X_0 + \sum_{i=1}^{t} \alpha^{t-i} \eta_i, \quad t = 0, ..., T. \tag{1.2}$$

We consider testing the hypothesis $H_0 : \alpha = 1$ under which X_t is a "random walk":

$$X_t = X_0 + \sum_{s=1}^{t} \Delta X_s = X_0 + \sum_{s=1}^{t} \eta_s.$$

This case is of particular interest in econometrics where, at least in the short term, many time series are believed to be (near) random walks (or, more generally, random walks plus stationary processes). It is often important to test this hypothesis, for instance against the alternative of stationarity, $|\alpha| < 1$. Here, with "stationarity" we do not mean that the process is stationary *conditional* on X_0, but rather that X_0 can for $|\alpha| < 1$ be given an (initional) distribution such that the process becomes stationary.

The random walk case is the interesting case where the time series is a martingale; future increments are independent of the past and are unpredictable. A random walk has the property that the "random shock" at time s, viz. $\Delta X_s = \eta_s$, has a permanent and constant effect on future levels X_t, $t \geq s$. In this sense the random walk case $\alpha = 1$ is the transition case between the stationary case $|\alpha| < 1$ where the effect of the shock η_s on future X_t, namely $\alpha^{t-s}\eta_s$, is dying exponentially as $t \to \infty$, and of the explosive case $\alpha > 1$ where this effect, $\alpha^{t-s}\eta_s$, is growing exponentially.

1.1.2 Testing the random walk hypothesis

This thesis analyses the asymptotic theory of test statistics for the random walk hypothesis $H_0 : \alpha = 1$. We start by defining the relevant test statistics which have been analysed for the first time by Dickey and Fuller (1979).

Different test statistics have been proposed. In our Gaussian model (1.1), the likelihood can be maximised analytically with respect to both parameters α and σ^2, yielding the maximum likelihood estimators

$$\hat{\alpha}_T := \frac{\sum_{t=1}^T X_{t-1}X_t}{\sum_{t=1}^T X_{t-1}^2}, \quad \hat{\sigma}_T^2 := \frac{1}{T}\sum_{t=1}^T \left(X_t - \hat{\alpha}_T X_{t-1}\right)^2. \tag{1.3}$$

Here $\hat{\alpha}_T$ is precisely the ordinary least squares ("OLS") estimator of α and $\hat{\sigma}_T^2$ differs from the OLS estimator of σ^2 only by the factor $(T-1)/T$. Two classical statistics for testing H_0 are obtained by the following two standardizations of $\hat{\alpha}_T$:

$$\tau_T := \frac{\hat{\alpha}_T - 1}{\hat{\sigma}_T\left(\sum_{t=1}^T X_{t-1}^2\right)^{-1/2}} \quad \text{and} \quad \kappa_T := T(\hat{\alpha}_T - 1).$$

Here, the "*t ratio*" τ_T is defined[1] by dividing $\hat{\alpha}_T - 1$ by an estimator of the standard deviation of $\hat{\alpha}_T$, and the "*normalised (coefficient) estimator*" κ_T is obtained by dividing $\hat{\alpha}_T - 1$ by its stochastic order under H_0, i.e. by T^{-1}.

The Gaussian model (1.1) also allows likelihood based testing. The "*(log) likelihood ratio*" test statistic can be calculated analytically and is found to be given by

$$L_T := -2\ln\left(\frac{\sup\left\{f_{\alpha,\sigma^2}(X_1,...,X_T|X_0)|\alpha = 1,\ \sigma^2 > 0\right\}}{\sup\left\{f_{\alpha,\sigma^2}(X_1,...,X_T|X_0)|\alpha \in \mathbf{R},\ \sigma^2 > 0\right\}}\right) = -T\ln\left(\frac{\hat{\sigma}_T^2}{\tilde{\sigma}_T^2}\right),$$

[1] A frequent alternative definition of the t ratio is obtained by replacing the maximum likelihood estimator $\hat{\sigma}_T^2$ by the OLS estimator of σ^2.

where $f_{\alpha,\sigma^2}(.|X_0)$ denotes the conditional density function of $X_1, ..., X_T$ given X_0. amd $\tilde{\sigma}_T^2$ is the maximum likelihood estimator of σ^2 under $H_0 : \alpha = 1$ (cf. Section 1.3.1). While L_T is suitable for testing H_0 versus the bilateral alternative $\alpha \neq 1$, a test versus the unilateral alternative $\alpha < 1$ (or versus $|\alpha| < 1$) can be based on the "*signed (log) likelihood ratio*" defined as:

$$W_T := \operatorname{sgn}(\hat{\alpha}_T - 1)\sqrt{L_T}.$$

1.1.3 Dickey-Fuller distributions

Usually, quantiles derived from the asymptotic (rather than the finite sample) distribution of the above test statistics are used to test H_0. Indeed, the asymptotic distribution of these statistics in many cases is a (very) good approximation of the finite sample distribution, particularly given the in econometrics often relatively large sample size; additional reasons why it is often convenient or even advisable to use asymptotic quantiles are given in Section 1.3.4

Each of the test statistics τ_T, κ_T, L_T and W_T indeed converge weakly in distribution, namely to non-standard, non-symmetric and in the case of τ_T, κ_T and W_T negatively biased distributions, which are known as *Dickey-Fuller distributions*. The statistics τ_T and W_T have the same limiting distribution (cf. Section 1.3.5), the square of which is the limiting distribution of L_T because $L_T = W_T^2$. Dickey-Fuller distributions can be expressed as functionals of a standard Brownian motion $(B(t))_{t\in[0,1]}$, viz.

$$\tau_T, W_T \xrightarrow{\mathcal{D}} \tau := \frac{R}{\sqrt{S}} \quad \text{and} \quad \kappa_T \xrightarrow{\mathcal{D}} \kappa := \frac{R}{S}, \tag{1.4}$$

where

$$R := \int_0^1 B(t)dB(t) = \frac{B(1)^2}{2} - \frac{1}{2} \quad \text{and} \quad S := \int_0^1 B(t)^2 dt. \tag{1.5}$$

This can be derived from Donsker's invariance principle, which states that an adequately rescaled and reparametrised[2] version of the random walk $X_T = X_0 + \sum_{t=1}^{T} \eta_T$ converges weakly in distribution to a Brownian motion (in the

[2]This involves normalizing by $T^{-1/2}$ and defining a (step) function $\mathcal{X} : [0,1] \mapsto \mathbf{R}$ by $\mathcal{X}(u) := T^{-1/2}X_t$ for $t/T \leq u < (t+1)/T$ where $t = 0, ..., T$.

function space of all real functions on $[0, 1]$ that are continuous from the right and have limits from the left, endowed with the supremum norm). In (1.5), the stochastic integral R was calculated using Itô's Lemma. For a proof of (1.4) under a more general error process η_t see Phillips (1987).

1.1.4 Why describe Dickey-Fuller distributions analytically?

The present section should present some motivations for describing the above asymptotic (Dickey-Fuller) distributions analytically as done in this thesis.

The analytical forms of the limiting distributions in (1.4) have been an open question for decades. These limiting distributions have been approximated by stochastic simulations (e.g. Fuller, 1976) and by numerical inversion techniques applied to White's (1958) limiting Laplace transform of a sufficient statistic (Evans and Savin (1981)). Also, Rao (1978) derives a complicated integral expression for the limiting density of τ_T (see Evans and Savin (1979) for corrections). The present thesis derives closed (i.e. integral-free, but not summation-free) expressions for the density and distribution functions of the limiting distributions in (1.4) – a task which has already been undertaken to some extent by Abadir (1993, 1995).

A first motivation is the aim of a better theoretical understanding of Dickey-Fuller distributions. This aim is reached only to a limited extent by this thesis since the derived analytical expressions show little apparent analytical structure.

A separate motivation is the numerical exploitation of the formulae, in particular for the derivation of quantiles. This approach contains some advantage over Monte-Carlo simulation. Firstly, our numerical methods reach very high standards of accuracy and efficiency. A second advantage over Monte-Carlo simulations is that, strictly speaking, only finite sample distributions can be simulated. Hence, based on simulations the properties of the limiting distribution can only be conjectured. In particular, quantiles of a limiting distribution can be conjectured by increasing the sample size T of simulations until the quantiles show a clear convergence. However, this lacks a mathematical proof. More formally, calling a the sought parameter of the limiting distribution (e.g. a quantile or a probability), a_T the corresponding parameter of the finite sample distribution, and $\hat{a}_T$ its simulation, the error $\hat{a}_T - a$ can be decomposed into the sum of the "simulation error" $\hat{a}_T - a_T$ and the deviation $a_T - a$ of the finite sample parameter from the limiting parameter. The rate of the convergence

$a_T \to a$ in the sense of a (reasonably strong) inequality $|a_T - a| \leq b_T$ is usually unknown.

Further, it might be seen as a disadvantage of simulations that the simulation error $\hat{a}_T - a_T$ is only known in the sense of an error distribution and hence of error probabilities or moments, but never in the sense of sure (non-trivial) error bounds. With positive probability, (very) high simulation errors may occur, even if the number of repetitions were chosen extremely high.

When a_T is a probability (such as $a_T := P(\tau_T \leq z)$), the standard deviation of $\hat{a}_T$ decreases only at the order $n^{-1/2}$ where n is the number of repetitions of the simulation. This implies practical boundaries to the achievable accuracy, although the commonly required accuracy usually falls within these boundaries. A problem, however, arises when $P(\tau_T \leq -z)$ or $P(\tau_T \geq z)$ (or the same for other test statistics) has to be simulated for very large values $z >> 0$: these probabilities then become very small, and the requirement of a certain *relative* precision[3] becomes hard to meet. For sufficiently high z, the required number of repetitions can not be computationally executed in reasonable time. However, this problem does not yet arise when calculating quantiles between the 1%- and the 99%-quantile.

1.2 Overview

As mentioned earlier, this thesis analyses the distributions of τ and κ arising in

$$\tau_T, W_T \xrightarrow{\mathcal{D}} \tau, \quad \kappa_T \xrightarrow{\mathcal{D}} \kappa \quad \text{and} \quad L_T \xrightarrow{\mathcal{D}} \tau^2$$

(cf. (1.4) and Section 1.3.5). The thesis is divided into a mathematical part (Chapter 2) and into a numerical part (Chapters 3 and 4). In Chapter 2 we prove expressions for the limiting (cumulative) distribution functions F_τ and F_κ which by differenciation yield formulae for the limiting probability density functions f_τ and f_κ. In the Chapters 3 and 4 we proceed with a numerical exploitation of the formulae for F_τ and F_κ, among others deriving highly accurate quantiles of τ and κ. Chapter 5 contains conclusive remarks. Some proofs and technical discussions are presented in the Appendix.

The derived results and, to an extent, also the methods are quite similar for τ and κ, and hence in the present qualitative overview let F represent either of the distribution functions F_τ and F_κ. Each derived expression for $F(z)$ is valid

[3]The relative error of $\hat{a}_T$ is $(\hat{a}_T - a_T)/a_T$.

either only for $z < 0$ or only for $z > 0$ and contains either one or two infinite series; in other words, $F(z)$ has the form

$$F(z) = \sum_{j=0}^{\infty} F_j(z) \quad \text{or} \quad F(z) = \sum_{j=0}^{\infty} \sum_{k=0}^{\infty} F_{jk}(z). \tag{1.6}$$

In this, the expression $F_j(z)$ respectively $F_{jk}(z)$ is integral-free but contains a special function. This special function is the incomplete gamma function $\Gamma(p, \zeta)$ in the case of $F_\tau(z)$ and the parabolic cylinder function $D_p(\zeta)$ in the case of $F_\kappa(z)$ (cf. Appendix A for special functions).

In Section 1.2.1 below we give an overview of Chapter 2 which consists of the derivation of our formulae of the kind of (1.6), followed in Section 1.2.2 by an overview of Chapters 3 and 4 which consist of the numerical treatment.

1.2.1 Overview of Chapter 2

Formulae of the type of (1.6) have already been derived by Abadir (1992, 1993, 1995). Our approach starts by giving rigorous proofs of some theoretic properties upon which the technical derivation of such formulae builds and which are implicitly assumed by Abadir. This is done in Sections 2.1 and 2.2. The (quite technical) derivation of new expressions of the form (1.6) for κ and τ follows in Sections 2.3 and 2.4. By differentiating the expressions of Sections 2.3 and 2.4 one can derive expressions for the densities of κ and τ, which is discussed in Section 2.5.

Abadir's and our derivations start by applying certain inversion integrals to the (joint) Laplace transform of the "limiting sufficient statistics" (R, S) appearing in (1.4) and (1.5). This limiting statistics is a limit in distribution of a certain sample statistics (R_T, S_T). The joint Laplace transform of (R, S) – the limit of that of (R_T, S_T) – has been calculated by White (1958). The main task of the theoretical preparations in Sections 2.1 and 2.2 is to prove the absolute continuity of (R, S) and hence the existence of a joint density $f_{R,S}$ of (R, S) on $\mathbf{R}^2$. This is a task of deducing properties of a distribution known only through its Laplace transform. To achieve this, some general criteria for distributions on $\mathbf{R}^n$ are derived in Section 2.2.

The results of Section 2.2 allow us to justify the use of the (Laplace) inversion integrals that form the basis of Abadir's and our derivations. The basic structure of these derivations is as follows. In order to calculate the occurring integrals analytically we develop the respective integrands into (converging) infinite series in such a way that the individual summands can now be integrated analytically. The interchangeability of summation and integration can usually be proven using the dominated convergence theorem, with one exception where a laborious proof is necessary since the integral is a Cauchy principal value integral. The termwise integrals are calculated in terms of special functions; as mentioned, this gives rise to an incomplete gamma function in expressions for τ respectively to a parabolic cylinder function in expressions for κ.

The derived series expressions for $F(z)$ compare as follows to those derived by Abadir.

Regarding τ, the author and Abadir are able to prove a closed formula only in the case of $z < 0$; this range of arguments contains all quantiles up to the 68%-quantile and hence in particular the quantiles needed to test against the alternatives $|\alpha| < 1$ (stationarity) and $\alpha < 1$. We derive a new formula with the advantage of containing a Leibniz series which yields a comfortable truncation criterion in the numerical implementation; indeed, in a Leibniz series the truncation error is in absolute value bounded above by the first omitted summand.

Regarding κ, we provide formulae for both cases $z < 0$ and $z > 0$, while Abadir does so only for $z < 0$. While Abadir's formula for $z < 0$ contains two infinite summations, one of our formulae for $z < 0$ contains a single infinite summation.

Using the known derivatives of the incomplete gamma and parabolic cylinder functions, our series expressions for the distribution functions of τ and κ can be differentiated so as to yield series expressions for the densities of τ and κ. The differentiation of a formula does not alter the number of infinite summations, but tends to result in a more complicated formula for the density. This is discussed in Section 2.5 which concludes Chapter 2.

1.2.2 Overview of Chapters 3 and 4

The numerical exploitation of our and Abadir's formulae for $F_\tau(z)$ and $F_\kappa(z)$ is treated in the Chapters 3 and 4. The provided techniques can be used for a highly accurate approximation of probabilities and quantiles.

A rigorous numerical approximation is possible only when knowing a truncation criterion for each series contained in a given formula. More explicitly, assume that $F(z)$ is written as, say, a single infinite series $F(z) = \sum_{j=0}^{\infty} F_j(z)$ and that one knows an inequality of the form

$$\left| \sum_{j=J+1}^{\infty} F_j(z) \right| \leq B(z, J),$$

where the bound $B(z, J)$ tends to 0 as $J \to \infty$. In the case of a Leibniz series, $B(z, J)$ can be set to be $|F_{J+1}(z)|$. Given some asked (absolute) precision $p > 0$, $F(z)$ should be approximated by $\sum_{j=0}^{J} F_j(z)$ where J is chosen (minimal) such that $B(z, J) \leq p$. The computational efficiency mainly depends on the rate of the convergence $B(z, J) \to 0$. Hence, inefficiency is either due to slow convergence of the series or to weakness of the bound $B(z, J)$.

Chapter 3 provides such bounds for most series occurring in the series expressions derived in Chapter 2. An exception is our expression for $F_\kappa(z)$ in the case $z > 0$; here, the author is unable to prove appropriate inequalities.

Building on the truncation error bounds of Chapter 3, the following Chapter 4 proceeds with a numerical discussion. The Sections 4.1 and 4.2 give some general programing advice, mainly aimed at preventing numerical instability and enhancing the efficiency. Among others, we provide ways of reordering summations so as to avoid multiple evaluations of (computationally expensive) terms, and ways of avoiding the parabolic cylinder function which is often not contained in software packages.

The Sections 4.3 and 4.4 report the author's specific observations and results of implementing approximations of $F_\tau(z)$ respectively of $F_\kappa(z)$. Besides reporting large tables of highly accurate quantiles, we discuss the specific levels of efficiency and accuracy reached by the different formulae. It is seen that most formulae allow a highly accurate approximation provided that z is not at the boundaries of the interval of validity of the respective formula. The exception is our formula for $F_\kappa(z)$ when $z > 0$; in this formula, where the author does not prove truncation error bounds that would allow a mathematically justified series truncation, numerical tests indicate that the series have very slow convergence rates.

1.3 Statistical context

This section, which is not essential for the understanding of the following chapters, describes the statistical context and background of unit root testing. The emphasis is on the one hand on comparing estimators and test statistics in autoregressive models with their counterparts in classical Gaussian regression analysis with deterministic regressors, and on the other hand on the special properties that estimators and test statistics in autoregressive models take on in the unit root case. Always guided by these two lines of emphasis, Sections 1.3.1 and 1.3.2 discuss estimators and test statistics, Section 1.3.3 considers their finite sample distributions, and Sections 1.3.4 and 1.3.5 consider asymptotic distributions.

The main conclusion of the distributional discussion of the Sections 1.3.3 to 1.3.5 is that, while in the classical Gaussian regression model with deterministic regressors the statistics have standard distributions, autoregressive models lead to non-standard distributions of statistics, and in the unit root case these distributions even stay non-standard asymptotically. This conclusion applies analogously to the Gaussian AR(1) model and to a wide range of more general models. For technical simplicity, the Sections 1.3.1 through 1.3.5 use the Gaussian AR(1) model as the vehicle of the discussion, as done so far in this chapter. In the final Section 1.3.6, however, we discuss unit root testing in more general models that still lead to the same asymptotic distributions analysed by this thesis. These model generalisations include increasing the autoregression order (Dickey and Fuller, 1979, 1981) and significantly relaxing the assumptions on the error process so as to allow for non-Gaussianity, heterogeneity and serial correlation (Phillips, 1987).

1.3.1 Estimation

We consider again the Gaussian AR(1) model (1.1), viz. the model

$$X_t = \alpha X_{t-1} + \eta_t, \quad t = 1, 2, ..., T,$$

with independent Gaussian errors $\eta_t \sim N(0, \sigma^2)$ and we condition on the initial value X_0. The expression of X_t in terms of X_0 and the errors $\eta_1, ..., \eta_t$ is given by (1.2). The joint (Gaussian) density of $(X_1, ..., X_T)$ can be factorised using that

$$(X_t | X_{t-1}, ..., X_0) \overset{\mathcal{D}}{=} (X_t | X_{t-1}) \sim N(\alpha X_{t-1}, \sigma^2), \quad t = 1, ..., T,$$

and hence is easily found to be given by

$$f_{\alpha,\sigma^2}(x_1, ..., x_T | x_0) := \frac{1}{(2\pi\sigma^2)^{T/2}} \exp\left\{ \frac{-1}{2\sigma^2} \sum_t (x_t - \alpha x_{t-1})^2 \right\}. \tag{1.7}$$

Maximization of the log density with respect to $(\alpha, \sigma^2) \in \mathbf{R} \times]0, \infty[$ as in Hamilton (1994, p. 122-123) yields the maximum likelihood estimators (1.3) for the parameters α and σ^2, viz. the estimators

$$\hat{\alpha}_T := \frac{\sum_{t=1}^T X_{t-1} X_t}{\sum_{t=1}^T X_{t-1}^2}, \quad \hat{\sigma}_T^2 := \frac{1}{T} \sum_{t=1}^T (X_t - \hat{\alpha}_T X_{t-1})^2,$$

whereas in the submodel with known $\alpha = \alpha_0 \in \mathbf{R}$ the variance is maximum likelihood estimated by

$$\tilde{\sigma}_T^2 := \frac{1}{T}\sum_{t=1}^{T}(X_t - \alpha_0 X_{t-1})^2 .$$

While often the maximisation of a log likelihood is possible only approximately, here the analytical forms of $\hat{\alpha}_T$, $\hat{\sigma}_T^2$ and $\tilde{\sigma}_T^2$ do exist essentially because of the nice likelihood function of a Gaussian autoregressive model. By substituting the above maximum likelihood estimators into the density (1.7), one obtains

$$\sup\left\{f_{\alpha,\sigma^2}(X_1,...,X_T|X_0)|\alpha \in \mathbf{R},\ \sigma^2 > 0\right\} = \frac{\exp\{-T/2\}}{(2\pi\hat{\sigma}^2)^{T/2}}, \tag{1.8}$$

$$\sup\left\{f_{\alpha,\sigma^2}(X_1,...,X_T|X_0)|\alpha = \alpha_0,\ \sigma^2 > 0\right\} = \frac{\exp\{-T/2\}}{(2\pi\tilde{\sigma}^2)^{T/2}}. \tag{1.9}$$

Now let us consider our model (1.1) as a regression model, with T equations where the present value X_t is regressed on the passed value X_{t-1}. Assume for a moment that in this regression model the regressor were deterministic, i.e. replace the stochastic regressor $(X_0,...,X_{T-1})'$ by a fixed vector $\mathbf{x} \in \mathbf{R}^T$. So, we are left with the classical regression model

$$\mathbf{Y} = \alpha\mathbf{x} + \eta, \quad \text{where } \mathbf{Y} := (X_1,...,X_T)',\ \eta := (\eta_1,...,\eta_T)'. \tag{1.10}$$

The least squares and maximum likelihood estimator of α is $\hat{\alpha} := (\mathbf{x}'\mathbf{x})^{-1}\mathbf{x}'\mathbf{Y}$. The assumption of a deterministic regressor $\mathbf{x}$ implies $\mathbf{Y} \sim N_T(\alpha\mathbf{x}, \sigma^2 I_T)$, and so $\hat{\alpha} \sim N(\alpha, V(\hat{\alpha}))$ with variance:

$$\begin{aligned} V(\hat{\alpha}) :=& (\mathbf{x}'\mathbf{x})^{-1}\mathbf{x}'\mathrm{Cov}(\mathbf{Y})((\mathbf{x}'\mathbf{x})^{-1}\mathbf{x}')' \\ =& (\mathbf{x}'\mathbf{x})^{-1}\mathbf{x}'(\sigma^2 I_T)\mathbf{x}(\mathbf{x}'\mathbf{x})^{-1} = \sigma^2(\mathbf{x}'\mathbf{x})^{-1}. \end{aligned} \tag{1.11}$$

A natural estimator of the variance (1.11) is $\hat{\sigma}_{\hat{\alpha}}^2 = \hat{\sigma}^2(\mathbf{x}'\mathbf{x})^{-1}$ where $\hat{\sigma}^2$ denotes the maximum likelihood estimator of σ^2.

Going back to our AR(1) model and bearing in mind the estimator $\hat{\sigma}_{\hat{\alpha}}^2$, we now define an analogous estimator for the variance of $\hat{\alpha}_T$:

$$\hat{\sigma}_{\hat{\alpha}_T}^2 := \hat{\sigma}_T^2 \left\{ \begin{pmatrix} X_0 \\ ... \\ X_{T-1} \end{pmatrix}' \begin{pmatrix} X_0 \\ ... \\ X_{T-1} \end{pmatrix} \right\}^{-1} = \hat{\sigma}_T^2 \left(\sum_{t=1}^{T} X_{t-1}^2 \right)^{-1} .$$

1.3.2 Testing the coefficient

Now we consider testing the null hypothesis $H_0 : \alpha = \alpha_0$ for some given $\alpha_0 \in \mathbf{R}$, both in the classical regression model (1.10) with deterministic regressors and in the AR(1) model.

First considering the classical regression model (1.10), H_0 is commonly tested via the t statistic, $t_\alpha := (\hat{\alpha} - \alpha_0)/\hat{\sigma}_{\hat{\alpha}}$ (notation as above). Accordingly, in our AR(1) model a t test of H_0 is based on the *t ratio* (or *t statistic*) with analogous definition:

$$\tau_T := \frac{\hat{\alpha}_T - \alpha_0}{\hat{\sigma}_{\hat{\alpha}_T}} = \frac{\hat{\alpha}_T - \alpha_0}{\hat{\sigma}_T \left(\sum_{t=1}^T X_{t-1}^2\right)^{-1/2}} = \frac{\sum_{t=1}^T X_{t-1}(X_t - \alpha_0 X_{t-1})}{\hat{\sigma}_T \sqrt{\sum_{t=1}^T X_{t-1}^2}}. \tag{1.12}$$

Often, the t statistic (in classical regression as well as in autoregression) is rather defined by replacing the maximum likelihood estimator of σ^2 by the least squares estimator (that differs by the factor $T/(T-1)$), or by the maximum likelihood estimator in the submodel H_0 (yielding the test statistic whose square is the *Lagrange multiplier* test statistic). But from the asymptotic perspective of this thesis all three definitions of the t statistic are equivalent since each variance estimator converges in probability to the same value σ^2.

The motivation for the t test statistic τ_T in an AR(1) is slightly less obvious than for the t statistic t_α in the model (1.10), because in the denominator $\hat{\sigma}^2_{\hat{\alpha}_T}$ is an often considerably biased estimator of the true variance $V(\hat{\alpha}_T)$ of the numerator $\hat{\alpha}_T - \alpha_0$. Only when testing a stationary hypothesis, i.e. when $|\alpha_0| < 1$, is there the asymptotic motivation that $\hat{\sigma}^2_{\hat{\alpha}_T}$ is an asymptotic variance of $\hat{\alpha}_T$ (more precisely, that $T^{-1}\hat{\sigma}^2_{\hat{\alpha}_T}$ consistently estimates the limiting variance of $T^{-1/2}(\hat{\alpha}_T - \alpha_0)$). However, the more important asymptotic argument, which is valid for *all* $\alpha_0 \in \mathbf{R}$, is that τ_T has a limiting distribution that does not depend on the unknown nuisance parameter σ^2, i.e. τ_T enables an asymptotically similar test of H_0.

In a likelihood-based approach (that can be motivated by the test theory of Neyman and Pearson), the test of H_0 against the *bilateral* alternative $\alpha \neq \alpha_0$ is based on the *(log) likelihood ratio*,

$$L_T := -2\ln\left(\frac{\sup\left\{f_{\alpha,\sigma^2}(X_1, ..., X_T|X_0)|\alpha = \alpha_0,\ \sigma^2 > 0\right\}}{\sup\left\{f_{\alpha,\sigma^2}(X_1, ..., X_T|X_0)|\alpha \in \mathbf{R},\ \sigma^2 > 0\right\}}\right) = -T\ln\left(\frac{\hat{\sigma}_T^2}{\tilde{\sigma}_T^2}\right), \tag{1.13}$$

where we used (1.8) and (1.9). In order to rewrite L_T in terms of the t ratio τ_T, we use a geometric property of least squares estimation. We illustrate the argument using the model (1.10) with deterministic regressors, $\mathbf{Y} = \alpha\mathbf{x}+\eta$. The least squares estimator $\hat{\alpha}$ is such that the vector $\mathbf{Y}$ is decomposed into the *orthogonal* sum of the "explained" component $\hat{\alpha}\mathbf{x}$ and the "residual" $\hat{\eta} := \mathbf{Y} - \hat{\alpha}\mathbf{x}$. Now, the orthogonality $\hat{\eta} \perp \mathbf{x}$ implies that $\hat{\eta} \perp v$ for all v in the span of $\mathbf{x}$, so that by Pythagoras' theorem $\|\hat{\eta}\|^2 = \|\hat{\eta} + v\|^2 - \|v\|^2$. Now note that the maximum likelihood estimator of σ^2 is precisely $\hat{\sigma}^2 = T^{-1}\|\hat{\eta}\|^2$, so that, letting $v := (\hat{\alpha} - \alpha_0)\mathbf{x}$, we deduce that

$$\begin{aligned}\hat{\sigma}^2 &= \frac{1}{T}\left(\|\hat{\eta} + (\hat{\alpha} - \alpha_0)\mathbf{x}\|^2 - (\hat{\alpha} - \alpha_0)^2\|\mathbf{x}\|^2\right) \\ &= \frac{1}{T}\|\mathbf{Y} - \alpha_0\mathbf{x}\|^2 - \frac{[\mathbf{x}'(\mathbf{Y} - \alpha_0\mathbf{x})]^2}{T\mathbf{x}'\mathbf{x}}.\end{aligned}$$

The first summand is precisely the maximum likelihood estimator of σ^2 under the hypothesis $\alpha = \alpha_0$. Applying this argument to our AR(1) model,

$$\hat{\sigma}_T^2 = \tilde{\sigma}_T^2 - \frac{\left[\sum_{t=1}^T X_{t-1}(X_t - \alpha_0 X_{t-1})\right]^2}{T\sum_{t=1}^T X_{t-1}^2} = \tilde{\sigma}_T^2 - \frac{\tau_T^2\hat{\sigma}_T^2}{T}.$$

Substituting this expression in (1.13), L_T is seen to be related to τ_T as follows:

$$L_T = -T\ln\left\{1 - T^{-1}\left(\frac{\tau_T\hat{\sigma}_T}{\tilde{\sigma}_T}\right)^2\right\}, \tag{1.14}$$

where $(\tau_T\hat{\sigma}_T/\tilde{\sigma}_T)^2$ is the Lagrange multiplier test statistic (cf. the comments following the definition (1.12) of τ_T).

A likelihood-based test of H_0 versus a *unilateral* alternatives (such as $\alpha < \alpha_0$) is possible by using the *signed (log) likelihood ratio* defined as:

$$W_T := \operatorname{sgn}(\hat{\alpha}_T - \alpha_0)\sqrt{L_T}.$$

While the tests based on τ_T, L_T and W_T can be formulated equivalently for a regression with deterministic regressors, the *estimator-based test* is specific to the autoregressive model. This test is based on the *normalised coefficient-estimator*,

$$\kappa_T := C(T)(\alpha_T - \alpha_0),$$

where the normalising factor $C(T)$ depends on α_0 and is defined as $T^{-1/2}$ if $|\alpha_0| < 1$, as T^{-1} if $|\alpha_0| = 1$, and as $|\alpha_0|^T$ if $|\alpha_0| > 1$. This normalisation ensures the convergence in distribution of κ_T to some non-degenerate limiting distribution (White, 1958). Provided that $|\alpha_0| \leq 1$, the limiting distribution does not depend on σ^2, meaning that an asymptotically similar test can be based on κ_T.

1.3.3 Finite sample distributions

We here briefly discuss that the nice distributional properties of statistics in the regression model with deterministic regressors are lost in the autoregressive model.

In the classical regression model (1.10), all of these distributions have got analytically known density functions. The coefficient estimator $\hat{\alpha}$ is unbiased and normally distributed. The estimator $\hat{\sigma}^2$ has a rescaled χ^2-distribution with $T-1$ degrees of freedom, and when multiplied by $T/(T-1)$ becomes unbiased but loses the maximum likelihood property. Under H_0, the t ratio t_α has a t distribution with $T-1$ degrees of freedom (rescaled by the factor $\sqrt{(T-1)/T}$ due to our choice of variance estimation in the denominator in t_α, cf. earlier remarks). Hence the distribution of t_α does not depend on unknown parameters, which allows similar testing. For greater detail, cf. Hamilton (1994, p. 202-205).

By contrast,.in the Gaussian AR(1) model none of the estimators $\hat{\alpha}_T$ and $\hat{\sigma}_T^2$ or of the test statistics τ_T, κ_T, L_T and W_T has standard analytical form. Simulations for several sample sizes T show that these distributions are non-symmetric, that the estimators are biased (Hamilton, 1994, p. 215-217), and that the test statistics τ_T and κ_T are negatively biased. However, asymptotically $\hat{\alpha}_T$ and $\hat{\sigma}_T^2$ are consistent.

1.3.4 Why use asymptotic quantiles?

Before discussing asymptotic distributions in the next subsection, we here first motivate the use of asymptotic quantiles in testing.

As already pointed out in Section 1.1.3, the asymptotic distribution of a test statistic is, at least in unit root testing, often a good approximation of its finite sample distribution, except for small sample size. Besides this, it is in many situations convenient or even necessary to use asymptotic quantiles, as is argued now.

The distribution of the errors η_t and the initial value X_0 affects the (finite sample) distribution of all test statistics τ_T, κ_T, L_T and W_T, but their limiting distributions are the same for a wide range of error processes and regardless of X_0 (except for κ_T when $|\alpha_0| > 1$), cf. Section 1.3.6. In practice, the error distribution is often little known. Even when it is known that the error process belongs to a certain parametric class, then the finite sample distribution of test statistics usually still depends on some unknown nuisance parameter(s), so that a similar test is usually impossible. For instance, the Gaussian AR(1) model (1.1) leaves unknown the error variance σ^2, and the finite sample test distributions depend on σ^2 unless $X_0 = 0$, as is seen later. For these reasons, the correct determination of finite sample quantiles (by Monte-Carlo simulation) may be difficult or impossible. In such situations, rather than using finite sample quantiles based on some more or less arbitrarily chosen error process, it is often preferable (and easier) to conduct a test based on quantiles of the limiting distribution. The latter is unambiguous, since the limiting distribution of each test statistic is independent of the nuisance parameter σ^2, allowing an asymptotically similar test. The imprecision of the used quantiles then results from the difference between the finite sample and the limiting distribution, rather than from a wrongly specified error distribution.

From a practical perspective, the use of finite sample quantiles may also have the inconvenience that tables may not be available for the particular needed error distribution, initial value X_0 and sample size T.

1.3.5 Asymptotic distributions

Now we come to the limiting distributions (under H_0) of τ_T, κ_T, L_T and W_T. It has already been discussed in Section 1.1.3 that in the unit root case of $\alpha_0 = 1$ all test statistics have non-standard, non-symmetric limiting ("Dickey-Fuller") distributions which can be represented in terms of functionals of a Brownian motion, cf. (1.4). These non-standard asymptotic distributions when $\alpha_0 = 1$ are an exception, as is seen in this section.

By methods of characteristic functions, White (1958, 1959) shows that for any $\alpha_0 \in \mathbf{R}$ both τ_T and κ_T have non-degenerate limiting distributions. Using Laplace inversions, he is able to determine the limiting distributions provided that $|\alpha_0| \neq 1$. Regarding τ_T, White (1959) finds $\tau_T \xrightarrow{\mathcal{D}} N(0,1)$ if $|\alpha_0| \neq 1$, as one might expect from comparing with t testing in the regression with deterministic regressors[4]. Regarding κ_T, White (1958) shows that $\kappa_T \xrightarrow{\mathcal{D}} N(0, 1 - \alpha_0^2)$ if $|\alpha_0| < 1$. If $|\alpha_0| > 1$, the limiting distribution is non-standard, except in the

[4]Indeed, the t distribution tends to $N(0,1)$ as the degree of freedom tends to ∞.

case $X_0 = 0$ where it is the Cauchy distribution; if $X_0 \neq 0$, the limiting density of κ_T has the form $f(z) = \sum_{k=0}^{\infty} c_k(1+z^2)^{-k-1}$, where the constants c_k depend on the ratio X_0/σ^2; the dependence on σ^2 shows that κ_T does not lend itself to an asymptotically similar test if $|\alpha_0| > 1$, i.e. if H_0 is an explosive hypothesis.

Now consider the likelihood-based test statistics L_T and W_T, and let α_0 be arbitrary again. Since $L_T = W_T^2$, the limiting distribution of L_T is the square of that of W_T (by the continuous mapping theorem, cf. Brockwell and Davis, 1998, p. 206). Moreover (as already mentioned for the case $\alpha_0 = 1$, cf. Section 1.1.3) W_T has the same limiting distribution as τ_T, so that if $|\alpha_0| \neq 1$ then $W_T \xrightarrow{\mathcal{D}} N(0,1)$ and $L_T \xrightarrow{\mathcal{D}} \chi^2(1)$. This asymptotic equivalence of W_T and τ_T can be shown as follows. First note that in (1.14) the term $T^{-1}\tau_T^2\hat{\sigma}_T^2/\tilde{\sigma}_T^2$ is of the stochastic order $O_P(T^{-1})$, because $\hat{\sigma}_T^2/\tilde{\sigma}_T^2 \xrightarrow{P} 1$ and $\tau_T = O_P(1)$. So, by a first order stochastic Taylor expansion of the logarithm in (1.14),

$$L_T = -T\left\{-T^{-1}\left(\frac{\tau_T\hat{\sigma}_T}{\tilde{\sigma}_T}\right)^2 + O_P(T^{-2})\right\} = \tau_T^2 + O_P(T^{-1}).$$

Hence, by stochastic Taylor expansion yields $\sqrt{L_T} = |\tau_T| + o_P(1)$, so that

$$W_T = \operatorname{sgn}(\hat{\alpha}_T - \alpha_0)\left(|\tau_T| + o_P(1)\right) = \operatorname{sgn}(\hat{\alpha}_T - \alpha_0)\,|\tau_T| + o_P(1) = \tau_T + o_P(1),$$

where we last used the definition of τ_T. In particular, W_T and τ_T have the same limiting distribution provided either variable converges in distribution (Brockwell and Davis, 1998, p. 205).

1.3.6 Extensions: Augmented Dickey-Fuller tests and Phillips-Perron tests

The importance of the analysed limiting distributions goes beyond the simple Gaussian AR(1) model discussed so far. Indeed, the restrictive assumptions on the distribution of X_t can be relaxed significantly without affecting the limiting distributions of the unit root tests τ_T and κ_T provided that their definitions are possibly adapted. We here briefly mention the two main approaches, namely that of (augmented) Dickey-Fuller tests and that of Phillips-Perron tests; for more detail the reader is referred to Appendix C which gives a concise overview of both approaches including the adapted definitions of τ_T and κ_T. The message is that the Dickey-Fuller distributions studied by this thesis are relevant to very general models provided that no deterministic level or trend is included.

In the case that an AR(1) model with serially uncorrelated disturbances is an inadequate representation of the data generating process, Dickey and Fuller (1979, 1981) propose to control for serial correlation by including higher order autoregressive terms[5], hence considering for some $p \geq 1$ the $AR(p)$ process X_t, $t = 0, ..., T$, satisfying:

$$X_t = \phi_1 X_{t-1} + ... + \phi_p X_{t-p} + \eta_t, \quad t = q, ..., T, \tag{1.15}$$

where η_t is an independent identically distributed sequence with mean 0 and finite fourth moment. In this model, Dickey and Fuller propose to test the hypothesis that the "lag polynomial" $1-\phi_1 z-...-\phi_p z^p$ possesses one "unit root" $z = 1$ and $p-1$ "stationary roots" $|z| > 1$. While this approach still supposes the specification of the autoregression order p, Phillips (1987) proposes a more general non-parametric approach by keeping an AR(1) equation,

$$X_t = \alpha X_{t-1} + \eta_t, \quad t = 1, 2, ..., \tag{1.16}$$

but allowing for very generally autocorrelated and heterogeneously distributed errors η_t.

While both generalisations do not affect the asymptotics of unit root tests (as redefined in Appendix C), the inclusion of a deterministic level parameter or of a linear trend parameter would affect limiting test distributions[6]. Hence the results of this thesis capture the generalisations (1.15) and (1.16), but do not apply to models with included deterministics.

1.4 Conventions

- See Appendix A for special functions
- See Appendix B for Laplace and Fourier transforms on $\mathbf{R}^n$, of Borel measures, integrable functions and random vectors.

General conventions:

[5] Dickey & Fuller (1981) and Phillips & Perron (1988) extend their respective studies to models (not part of this thesis) that also contain a deterministic level or linear trend.

[6] These cases are treated by Dickey & Fuller (1981) and Phillips & Perron (1988).

- $a := x$ means that the symbol a is defined as the expression x.
- $\mathbf{N} := \{0, 1, 2, ...\}$, $\mathbf{Z} := \{0, \pm 1, \pm 2, ...\}$ $\mathbf{R}_+ := (0, \infty)$, $\mathbf{R}_- := (-\infty, 0)$.
- $(-)^n := (-1)^n \quad$ for all $n \in \mathbf{Z}$.

Probability theory conventions:

- For any random variable Z in $\mathbf{R}$ or $\mathbf{R}^n$ we denote by $F_Z(z)$ its (cumulative) distribution function and (if existent) by $f_Z(z)$ its (probability) density function.
- $Y_T \xrightarrow{P} Y$ denotes the convergence in probability[7] of the the random variable Y_T to the (possibly constant) random variable Y as $T \to \infty$.
- $Y_T \xrightarrow{\mathcal{D}} L$ denotes the (weak) convergence of the distribution of the random variable Y_T to L if L is a distribution, respectively to the distribution of L if L is a random variable.
- $Y \stackrel{\mathcal{D}}{=} L$ means that the random variable Y has the distribution L.
- For a sequence of random variables Y_T and a deterministic sequence a_T the *stochastic order* notation is defined as follows[7] (Brockwell and Davis, 1991, p. 199):

  $Y_T = o_P(a_T)$ if and only if $Y_T/a_T \xrightarrow{P} 0$;

  $Y_T = O_P(a_T)$ if and only if Y_T/a_T is *bounded in probability*, i.e. for all $\varepsilon > 0$ there exists a $B(\varepsilon) > 0$ such that $P(|Y_T/a_T| > B(\varepsilon)) < \varepsilon$ for all T.

A complex analysis convention

- When calling a function f of a *real* variable s (such as a density function) "holomorphic" in s, we mean that f possesses an extension to a function on a complex neighbourhood of s which is holomorphic in s.

[7]The symbol "P" stands for the probability measure on the σ-algebra over the underlying probability space Ω.

Chapter 2

Series for Dickey-Fuller Distributions

This chapter begins with the analysis of the limiting joint Laplace transform of a sufficient statistic for our Gaussian model, calculated by White (1958). Section 2.1 states White's result and a few consequences, and then Section 2.2 proceeds with the derivation of general criteria on distribution functions on $\mathbf{R}^n$, which will imply the absolute continuity of the limiting distribution of the sufficient statistic. In the sections 2.3 and 2.4 we derive our closed expressions for the limiting distribution functions of the two considered test statistics. We treat the normalised coefficient estimator κ_T first (cf. Section 2.3) since the discussion is slightly less involved than for the t statistic τ_T (cf. Section 2.4).

2.1 The Laplace transform of the limiting sufficient statistics (R, S)

Consider the Gaussian AR(1) model (1.1). All probabilities are conditional on X_0. We consider testing the random walk hypothesis $H_0 : \alpha = 1$. The test statistics κ_T and τ_T can be written as $\kappa_T = R_T/S_T$ and $\tau_T = R_T/(\hat{\sigma}_T\sqrt{S_T})$, where

$$R_T := T^{-1}\sum_t (X_t - X_{t-1})X_{t-1} \quad \text{and} \quad S_T := T^{-2}\sum_t X_{t-1}^2.$$

Since only the distributions of κ_T and τ_T interest us, we may assume that $\sigma^2 = 1$ after modifying X_0. The reason is that κ_T and τ_T remain unchanged when each occurring $X_0, ..., X_T$ is divided by σ, so that κ_T and τ_T are functions of $X_0/\sigma, ..., X_T/\sigma$; and by (1.2) the distribution of each X_t/σ (and hence that of κ_T and τ_T) depends on the pair X_0, σ^2 only through the ratio X_0/σ. So one of X_0, σ^2 can be restricted; more precisely, we replace the pair X_0, σ^2 by the pair $X_0/\sigma, 1$ without affecting the distributions of κ_T and τ_T.

In the submodel where σ^2 is set to 1 and α is the only parameter, the statistics (R_T, S_T) is sufficient, while in the original model (R_T, S_T, σ_T^2) is sufficient. While the joint density of (R_T, S_T) is analytically unknown, White (1958) is able to calculate its joint Laplace transform[1], $E\left\{\exp\left(-uR_T - vS_T\right)\right\}$ and derives the limit for $T \to \infty$. His result can be stated as follows[2].

Theorem 2.1 *(White, 1958, p. 1193) Let $\alpha = \sigma^2 = 1$. The Laplace transform of (R_T, S_T) converges in a neighbourhood of the origin $(u, v) = (0, 0) \in \mathbf{R}^2$. So, there exists a random vector (R, S) in $\mathbf{R}^2$ such that $(R_T, S_T) \xrightarrow{\mathcal{D}} (R, S)$, and in a neighbourhood of the origin (R, S) possesses a Laplace transform that is given by:*

$$\begin{aligned} E\{\exp(-uR - vS)\} &= \lim_{T\to\infty} E\left\{\exp(-uR_T - vS_T)\right\} \\ &= e^{u/2}\left(\cosh\sqrt{2v} + \frac{u}{\sqrt{2v}}\sinh\sqrt{2v}\right)^{-1/2}. \end{aligned} \tag{2.1}$$

[1]This is possible as follows (where we assume for simplicity that $X_0 = 0$). Both R_T and S_T are quadratic forms in Gaussian variables. If A_T and B_T denote the $T \times T$-matrices representing the quadratic forms R_T resp. S_T, and if C_T denotes the $T \times T$-covariance-matrix of the Gaussian vector $(X_1, ..., X_T)'$ given X_0, then $\mathbf{E}\left\{\exp\left(-uR_T - vS_T\right)\right\}$ equals

$$[2\pi \det(C_T)]^{-T/2} \int_{\mathbf{R}^T} \exp\left(-\frac{1}{2}x'(C_T^{-1} + 2uA_T + 2vB_T)x\right) dx,$$

and hence, using a known integration formula (Cramér (1946, p. 120),

$$\mathbf{E}\left\{\exp\left(-uR_T - vS_T\right)\right\} = \det(C_T)^{-T/2} \det\left(C_T^{-1} + 2uA_T + 2vB_T\right)^{-1/2}.$$

While $\det(C_T)$ is easily seen to equal 1, the second determinant can be calculated via a difference equation.

[2]Minor differences result from the fact that White in fact uses the *moment generating function* $\mathbf{E}\left\{\exp\left(uR_T + vS_T\right)\right\}$ (note the changed sign in the exponential function), and that his definitions of R_T and S_T differ by the factor $\sqrt{2}$ respectively 2.

From the continuous mapping theorem and $\sigma_T^2 \xrightarrow{P} 1$ we deduce the following corollary (which holds for general σ^2 by the earlier remark).

Corollary 2.2 *Under $H_0 : \alpha = 1$, we have $\tau_T \xrightarrow{\mathcal{D}} \tau := R/\sqrt{S}$ and $\kappa_T \xrightarrow{\mathcal{D}} \kappa := R/S$, where (R, S) is as in Theorem 2.1.*

Note that the Laplace transform in Theorem 2.1 is independent of X_0 and σ^2, and hence so are the distributions of τ and κ under H_0.

PROOF OF THEOREM 2.1. The convergence of the Laplace transform is shown by White (1958). The convergence in distribution follows from the continuity theorem for Laplace transforms respectively moment generating functions[3]. Alternatively, one can argue using characteristic functions: Since the characteristic function $E\left\{\exp(iuR_T + ivS_T)\right\}$ converges for all $(u, v) \in \mathbf{R}^2$ and since the limit is continuous in $(u, v) = (0, 0)$, the vector (R_T, S_T) converge in distribution by the continuity theorem for characteristic functions. **QED**.

Alternatively to White's Fourier approach, the convergence in distribution (for $\alpha = 1$) can be deduced from Donsker's invariance principle which provides an expression of (R, S) as a function of a standard Brownian motion $(B(t))_{t\in[0,1]}$:

$$
\begin{aligned}
(R_T, S_T) \xrightarrow{\mathcal{D}} (R, S) &:= \left(\int_0^1 B(t)dB(t), \int_0^1 B(t)^2 dt \right) \\
&= \left(\frac{1}{2}B(1)^2 - \frac{1}{2}, \int_0^1 B(t)^2 dt \right) \qquad (2.2)
\end{aligned}
$$

where $\int_0^1 B(t)dB(t)$ is an (Itô) stochastic integral (e.g. Phillips, 1987). This implies $P(R > -1/2) = 1$ and $P(S > 0) = 1$.

The individual Laplace transforms of R and S are obtained by putting $v = 0$ respectively $u = 0$ in (2.1):

$$
E\left\{\exp(-uR)\right\} = e^{u/2}\left(1+u\right)^{-1/2}, \; E\left\{\exp(-vS)\right\} = \cosh^{-1/2}\sqrt{2v}.
$$

The first expression is the Laplace transform of a $\chi^2(1)/2 - 1/2$ distributed variable, matching (2.2). From the second expression, we now deduce properties of the distribution of S:

[3]See Curtis (1942) for the continuity theorem for one-dimensional Laplace transforms, and Jensen & Nielsen (1996) for the generalisation to multi-dimensional Laplace transforms.

Corollary 2.3 *The limiting variable S possesses a density function $f_S(s)$ that is a Schwartz function, i.e. is infinitely many times differentiable with derivative $f_S^{(k)}(s)$ of order $o(|s|^{-n})$ as $|s| \to \infty$, for any fixed $k, n \in \mathbf{N}$. Moreover, $f_S(s) = 0$ for $s \leq 0$.*

Before we prove this corollary, note that what is surprising is that, although $f_S(s)$ cannot be holomorphic in each $s \in \mathbf{R}$ (since to the left of the origin $f_S(s)$ becomes the function equal to 0), all derivatives $f_S^{(k)}(s)$ exist, also in $s = 0$, implying a "smooth transition" at the origin. Since in $s = 0$ all left-side-derivatives of $f_S(s)$ are 0, all right-side-derivatives are 0 too, and hence the distribution of S dies out very fast at both extremities:

Corollary 2.4 *For all $n \in \mathbf{N}$,*
(a) as $s \downarrow 0$, $f_S(s) = o(s^n)$ and hence $F_S(s) = o(s^n)$,
(b) as $s \uparrow \infty$, $f_S(s) = o(s^{-n})$ and hence $F_S(s) = 1 - o(s^{-n})$.

By contrast, consider a standard density such as the $\chi^2(m)$ density. The latter equals $\{\Gamma(m/2)2^{m/2}\}^{-1}s^{m/2-1}e^{-s/2}$ when $s > 0$ and 0 when $s \leq 0$; for $m \leq 2$ this density is discontinuous in $s = 0$; for odd $m > 2$ not all right-side-derivatives in $s = 0$ exist, and for even $m > 2$ all right-side derivatives in $s = 0$ exist, but not all of them are 0.

Proof of Corollary 2.3. The Fourier transform of S is $E\{\exp(-ivS)\} = \cosh^{-1/2}\sqrt{2iv}$, where the relevant holomorphic branch of this multifunction is defined by taking the value 1 in $v = 0$. We claim that this is a Schwartz function. Note first that a Taylor expansion of cosh shows that $\cosh\sqrt{2iv}$ is holomorphic for all $v \in \mathbf{R}$ (in fact for all $v \in \mathbf{C}$). Since $\cosh\sqrt{2iv} \neq 0$ for all $v \in \mathbf{R}$, it follows that $E\{\exp(-ivS)\}$ is holomorphic in each $v \in \mathbf{R}$. In particular, all derivatives of $E\{\exp(-ivS)\}$ exist. From

$$E\{\exp(-ivS)\} = \sqrt{2}e^{-\sqrt{2iv}/2}\left[1 + e^{-2\sqrt{2iv}}\right]^{-1/2}$$

it is clear that each derivative $D^k E\{\exp(-ivS)\}$ has the form of a linear combination of terms of the form $(2iv)^{1/2+a}e^{-(1+4b)\sqrt{2iv}/2}\left(1 + e^{-2\sqrt{2iv}}\right)^{-1/2-c}$ with $a \in \mathbf{Z}$ and $b, c \in \mathbf{N}$, each of which is indeed of the order $o(|v|^{-n})$ as $|v| \to \infty$.

Now, call $\mathfrak{S}(\mathbf{R})$ the "*Schwartz-space*" of all (complex-valued) Schwartz functions on $\mathbf{R}$. Fourier transformation, if restricted to functions in $\mathfrak{S}(\mathbf{R})$, establishes a bijective (linear) transformation from $\mathfrak{S}(\mathbf{R})$ onto itself (e.g. Werner, 1995, p. 168). Hence there is a (unique) Schwartz function $g \in \mathfrak{S}(\mathbf{R})$ whose Fourier transform is $E\{\exp(-ivS)\}$. By the uniqueness theorem for Fourier transforms of Borel measures (e.g. Petersen, 1983, p. 74, Corollary 3.9), the (absolutely continuous[4]) Borel measure defined by the density function g must be the probability distribution of S. **QED**.

2.2 Some general propositions on multivariate distributions and the absolute continuity of (R, S)

The absolute continuity[4] of the joint distribution of (R, S), which seems nearly as plausible as that of the individual R or S (for S cf. Corollary 2.3) and is implicitly assumed in the literature, deserves an explicit proof. We now derive criteria of general interest for the *continuity*[5] (Proposition 2.6) and for the *absolute continuity*[4] (Propositions 2.5 and 2.8) of probability distributions on $\mathbf{R}^n$. These results will enable us to prove first the continuity of (R, S) (cf. Section 2.2.1) and later the absolute continuity of (R, S) (cf. Section 2.2.2).

2.2.1 Two general propositions and the continuity of (R, S)

This section relies on arguments of Fourier Analysis. See Appendix B for the definitions of Laplace and Fourier transforms of functions and Borel measures. In this and the following subsection let $n \in \{1, 2, ...\}$.

In a slight digression we first generalise a known criterion for the absolute continuity[4] of a probability distribution on $\mathbf{R}^n$ (Propositions 2.5), cf. Dietrich (2002c). As this criterion is not applicable to the distribution of (R, S), we then prove a second (related) general result (Proposition 2.6), cf. Dietrich

[4]A probability distribution P on $\mathbf{R}^n$ is called "absolutely continuous" (with respect to the Lebesgue measure λ^n on $\mathbf{R}^n$) if $P(A) = 0$ for all null-sets $A \subset \mathbf{R}^2$, i.e. all (measurable) sets $A \subset \mathbf{R}^2$ of Lebesgue-Borel measure $\lambda^n(A) = 0$. The theorem of Radon-Nikodym then implies the existence of a density $f : \mathbf{R}^n \mapsto \mathbf{R}$ for P (with respect to the Lebesgue-Borel measure λ^n), i.e. $P(A) = \int_A f(x)dx$ for all measurable sets $A \subseteq \mathbf{R}^n$.

[5]A probability distribution on $\mathbf{R}^n$ is *continuous* if its cumulative distribution function is continuous on $\mathbf{R}^n$. This requirement is weaker than that of absolute continuity.

(2002c); the latter result does apply to (R, S) but is a criterion merely for (not necessarily absolute) continuity[5] of a distribution. Both criteria are based on Laplace transforms and are proven using Fourier Transform Theory.

It is known (e.g. Breiman (1992, p. 178) or Lukacs (1960, p. 40)) that if P is a probability measure on $\mathbf{R}$ whose Fourier transform,

$$\hat{P}(u) := \int_{\mathbf{R}} \exp(-iux)dP(x),$$

is (absolutely) integrable over $\mathbf{R}$, then P is absolutely continuous and possesses a continuous density f to be retrieved via:

$$f(x) = \frac{1}{2\pi}\int_{\mathbf{R}} \exp(iux)\hat{P}(u)du, \quad \forall x \in \mathbf{R}.$$

However, not all absolutely continuous distributions have Fourier transforms of this kind, the obvious counterexample being when the density has a discontinuity such for the $\chi^2(1)$ distribution. In such cases, at least the *continuity* (rather than the *absolute continuity*) of the distribution can often be deduced using the criterion of Proposition 2.6 below.

First, let us formulate the mentioned known criterion more generally for probability distributions P on (the Borel sets of) $\mathbf{R}^n$ and for the *Laplace* transform.

$$\bar{P}(a) := \int_{\mathbf{R}^n} \exp(-a'x)dP(x). \tag{2.3}$$

Proposition 2.5 *If the Laplace integral $\bar{P}$ of an arbitrary probability distribution P on $\mathbf{R}^n$ exists[6] in $q \in \mathbf{R}^n$ (and hence on the affine subspace $q + (i\mathbf{R})^n$), and if $\int_{\mathbf{R}^n} \left|\bar{P}(q + ia)\right| da < \infty$, then P possesses an everywhere continuous density f which can be retrieved via:*

$$\begin{aligned} f(x) &= \frac{1}{(2\pi i)^n}\int_{q+(i\mathbf{R})^n} \exp(a'x)\bar{P}(a)da \\ &= \exp(q'x)\frac{1}{(2\pi)^n}\int_{\mathbf{R}^n} \exp(ia'x)\bar{P}(q + ia)da \end{aligned} \tag{2.4}$$

for all $x \in \mathbf{R}^n$. Moreover, $f(x) = o\{\exp(q'x)\}$ as $\|x\|_2 \to \infty$.

[6]Existence is meant in the sense of (absolute) Lebesgue-integrability.

Here, $\|x\|_2 := \sqrt{x_1^2 + ... + x_n^2}$ for all $x = (x_1, ..., x_n) \in \mathbf{R}^n$, and the relation $f(x) = o\{\exp(q'x)\}$ as $\|x\|_2 \to \infty$ means that

$$\lim_{\|x\|_2 \to \infty} \{\exp(-q'x) f(x)\} = 0;$$

note that this does not simply follow from the assumed existence (i.e. finiteness) of $\bar{P}(q) = \int_{\mathbf{R}^n} \exp(-q'x) f(x) dx$.

PROOF. If P possesses a density given by (2.4), then $f(x)$ is continuous and satisfies $f(x) = o\{\exp(q'x)\}$ as $\|x\|_2 \to \infty$, because the Fourier integral $\exp(-q'x)f(x) = \int_{\mathbf{R}^n} \exp(ia'x)\bar{P}(q+ia)da$ is continuous and vanishes at infinity by the theorem of Riemann-Lebesgue (Petersen, 1983, p. 67, 74).

We now prove the existence of a density given by (2.4). We will see that the statement can be reformulated in terms of Fourier transforms and follows from a deep result of Fourier Analysis, namely that

$$g(x) = (2\pi)^{-n} \hat{\hat{g}}(-x), \tag{2.5}$$

where g is any *tempered distribution*, i.e. generalised function in the sense of a linear continuous functional on the Schwartz space $\mathfrak{S}(\mathbf{R}^n)$. For reference, see for instance Donoghue (1969, p. 134-149), or Petersen (1983, Section 2.7). In the space $\mathfrak{S}'(\mathbf{R}^n)$ of tempered distributions are (among others) embedded all bounded Borel measures (in particular $L^1(\mathbf{R}^n)$), and the Fourier transformation on $\mathfrak{S}'(\mathbf{R}^n)$ is an extension of the Fourier transformation on the bounded Borel measures Q given by the Fourier integral

$$\hat{Q}(u) := \int_{\mathbf{R}^n} \exp(-iu'x) dQ(x). \tag{2.6}$$

In the particular case that in (2.5) g is a bounded Borel measure Q, the first transform $\hat{g} = \hat{Q}$ is given by the Fourier integral (2.6) while the second transform $\hat{\hat{g}} = \hat{\hat{Q}}$ is in general the Fourier transform of the *tempered distribution* $\hat{Q}$ since $\hat{Q}$ need not be (absolutely) integrable over $\mathbf{R}^n$. Now let Q be the Borel measure $Q := \exp(-q'x)P$ with Fourier transform $\hat{Q}(a) = \bar{P}(q + ia)$. By assumption, this Borel measure (which is bounded since $Q(\mathbf{R}^n) = \hat{Q}(0) < \infty$) has (absolutely) integrable Fourier transform: $\int_{\mathbf{R}^n} |\hat{Q}(ia)| da < \infty$; hence even the second transform $\hat{\hat{g}} = \hat{\hat{Q}}$ is given by Fourier integration. So, in (2.5) we know that $\hat{\hat{g}}$ and hence g are functions in the standard sense (respectively absolutely continuous distributions), and by (2.5) a density for $g = Q$ is given by the Fourier integral $f_Q(x) := (2\pi)^{-n} \int_{\mathbf{R}^n} \exp(ia'x)\hat{Q}(a)da$. Hence the probability measure $P = \exp(q'x)Q$ is also absolutely continuous and its density $f(x) = \exp(q'x)f_Q(x)$ becomes (2.4). **QED**.

Proposition 2.5 does *not* apply to the distribution $P_{R,S}$ of (R,S). As is easily seen from White's Laplace transform $\bar{P}_{R,S}(u,v)$ (Theorem 2.1), if v is fixed then $|\bar{P}_{R,S}(u,v)|$ is of the order as high as $|u|^{-1/2}$ as $|u| \to \infty$ in $\mathbf{C}$, and hence the relevant absolute integral in Proposition 2.5 is infinite.

We now derive a criterion for continuity[5] of distributions which can be used either in (rare) cases of continuous but not absolutely continuous distributions or in many cases of absolutely continuous distributions for which Proposition 2.5 does not apply such as when the density has a discontinuity. The criterion is based on the Laplace transform of a *(cumulative) distribution function*[7] $F : \mathbf{R}^n \mapsto R$,

$$\bar{F}(a) := \int_{\mathbf{R}^n} \exp(-a'x)F(x)dx, \tag{2.7}$$

as opposed to the Laplace transform (2.3) of the associated probability measure $P := dF$. The transforms $\bar{F}$ and $\bar{P}$ are related through:

$$\bar{F}(a_1, ..., a_n) = \frac{1}{a_1 a_2 \cdots a_n} \bar{P}(a), \quad \text{where } a = (a_1, ..., a_n); \tag{2.8}$$

more precisely, if $\bar{F}$ exists in $a \in \mathbf{C}^n$ (with $\operatorname{Re} a_i > 0 \ \forall i$), then so does $\bar{P}$, and one has (2.8).

Proposition 2.6 *If the Laplace integral $\bar{F}$ of an arbitrary distribution function F (to some probability measure) on $\mathbf{R}^n$ exists*[6] *in $q \in \mathbf{R}^n$ (and hence on the affine subspace $q + (i\mathbf{R})^n$), and if $\int_{\mathbf{R}^n} \left|\bar{F}(q + ia)\right| da < \infty$, then F is everywhere continuous and can be retrieved via:*

$$\begin{aligned} F(x) &= \frac{1}{(2\pi i)^n} \int_{q+(i\mathbf{R})^n} \exp(a'x)\bar{F}(a)da \\ &= \exp(q'x)\frac{1}{(2\pi)^n} \int_{\mathbf{R}^n} \exp(ia'x)\bar{F}(q + ia)da \end{aligned} \tag{2.9}$$

for all $x \in \mathbf{R}^n$. Moreover, $F(x) = o\{\exp(q'x)\}$ as $\|x\|_2 \to \infty$.

---

[7]The term "(cumulative) distribution function" is here always used with respect to a *probability* measure P on $\mathbf{R}^n$. It is defined by $F(x_1, ..., x_n) := P((-\infty, x_1] \times ... \times (-\infty, x_n])$, is continuous from above and tends to 0 and 1 as $(x_1, ..., x_n)$ tends to $(-\infty, ..., -\infty)$ respectively to $(\infty, ..., \infty)$.

PROOF. Consider the function

$$f(x) := \exp(-q'x)F(x) \tag{2.10}$$

which has Fourier transform given by $\hat{f}(a) = \bar{F}(q+ia)$. Using the same argument than in the proof of Proposition 2.5, the (absolute) integrability of $\hat{f}$ implies that f can be retrieved from $\hat{f}$ via the Fourier (inversion) integral; more precisely, f is almost surely identical to the continuous Fourier inverse

$$g(x) := \frac{1}{(2\pi)^n}\int_{\mathbf{R}^n} \exp(ia'x)\hat{f}(a)da = \frac{1}{(2\pi)^n}\int_{\mathbf{R}^n} \exp(ia'x)\bar{F}(q+ia)da.$$

We have to show that $f(x) = g(x)$ for *all* $x \in \mathbf{R}^n$, which by (2.10) implies the continuity of F and the claimed representation for F. Let $x \in \mathbf{R}^n$. We show that $f(x) = g(x)$. Since f and g coincide almost everywhere there exists a sequence $(x_n)_{n\in\mathbf{N}}$ in $\mathbf{R}^n$ such that $x_n \downarrow x$ and $f(x_n) = g(x_n)$ for all $n \in \mathbf{N}$.By the continuity of g we have $g(x) = \lim_{n\to\infty} g(x_n)$, and by the continuity *from above* of the distribution function F and hence of f we have $f(x) = \lim_{n\to\infty} f(x_n)$, implying that $f(x) = g(x)$. **QED**.

Note that the inversion formulae of both Propositions are (proper) Lebesgue-integrals which (by Fubini's theorem) can be decomposed into n one-dimensional Laplace inversion integrals, the order being arbitrary. For instance, in Proposition 2.6, when $n = 2$ and putting $q = (q_1, q_2)'$ and $x = (x_1, x_2)'$,

$$\begin{aligned} F(x_1,x_2) &= \frac{1}{2\pi i}\int_{q_2+i\mathbf{R}} da_2\, e^{x_2a_2}\frac{1}{2\pi i}\int_{q_1+i\mathbf{R}} e^{x_1a_1}\bar{F}(a_1,a_2)da_1 \\ &= \frac{1}{2\pi i}\int_{q_1+i\mathbf{R}} da_1\, e^{x_1a_1}\frac{1}{2\pi i}\int_{q_2+i\mathbf{R}} e^{x_2a_2}\bar{F}(a_1,a_2)da_2. \end{aligned} \tag{2.11}$$

Before applying Proposition 2.6 to $F_{R,S}$, some remarks to this proposition are appropriate:

1. Although continuous, F need not be absolutely continuous and hence need not possess a density.

2. The Laplace transform of a distribution function can only exist in points $q \in \mathbf{R}^n$ with only positive coordinates, i.e. q must lay in $\mathbf{R}^n_+$. A class of distribution functions F for which $\bar{F}(q)$ exists *in every* $q \in \mathbf{R}^n_+$ is the class of distribution functions F that die outside some set of the form $B := [y_1,\infty) \times \ldots \times [y_n,\infty)$ where $(y_1,\ldots,y_n) \in \mathbf{R}^n$, i.e. B has probability 1: indeed, if $F(x) = 0$ for $x \notin B$ the Laplace integral $\bar{F}(q)$ is in fact an integral over B rather than $\mathbf{R}^n$

and exists in each $q \in \mathbf{R}_+^n$. This situation is given for the distribution function $F_{R,S}$ since (R,S) falls into $(-1/2,\infty) \times \mathbf{R}_+$ with probability 1.

3. In practice, Proposition 2.6 should apply to most Laplace transforms $\bar{F}$ – if existent in some $q \in \mathbf{R}^n$ – of *absolutely* continuous distribution functions F, so that at least the continuity of F can be derived. Indeed, if $\bar{F}$ exists on $q + (i\mathbf{R})^n$ (where $q \in \mathbf{R}_+^n$) then the Laplace transform $\bar{P}$ of $P := dF$ also exists on $q + (i\mathbf{R})^n$, and by the theorem of Riemann-Lebesgue (Petersen, 1983, p. 67, 74) the function $a \mapsto \bar{P}(q+ia)$ from $\mathbf{R}^n \mapsto \mathbf{C}$ vanishes as $\|a\|_2 \to \infty$; hence it should usually be (but not always is) the case that the function

$$a \mapsto \bar{F}(q+ia) = \frac{1}{(q_1+ia_1)(q_2+ia_2)\cdots(q_n+ia_n)}\bar{P}(q+ia)$$

is absolutely integrable over $\mathbf{R}^n$.

4. One might be tempted to deduce even the absolute continuity of F by differentiating under the integral in (2.9). This, however, is allowed only when the differentiated integrand is absolutely integrable, which (using (2.8)) is precisely when already Proposition 2.5 applies. However, if the integral in (2.9) can be calculated analytically then a proof of absolute continuity and the derivation of a density is often possible by differentiating the (integral-free) expression for $F(x)$. Alternatively, after decomposing the integral (2.9) into one-dimensional inversions as in (2.11) and analytically solving *some* of these inversions, it may be that the absolute continuity and a density expression now are derivable since differentiation under the (remaining) integrals may now be allowed. Precisely this is done with $F_{R,S}$ in the remainder of Section 2.2.

By Remark 2, the distribution function $F_{R,S}$ of the limiting statistic (R,S) possesses a Laplace transform $\bar{F}_{R,S}(u,v)$ in each $(u,v) \in \mathbf{C}^2$ satisfying $\operatorname{Re} u > 0$ and $\operatorname{Re} v > 0$, and by the remark made in front of Proposition 2.6

$$\text{(2.12)}\quad \bar{F}_{R,S}(u,v) = \frac{1}{uv}\bar{P}_{R,S}(u,v) = \frac{1}{uv}e^{u/2}\left(\cosh\sqrt{2v} + \frac{u}{\sqrt{2v}}\sinh\sqrt{2v}\right)^{-1/2},$$

where the formula of Theorem 2.1 is used (extended analytically to any $\operatorname{Re} u > 0$ and $\operatorname{Re} v > 0$). We now show that $\bar{F}_{R,S}$ satisfies the condition of Proposition 2.6, and more precisely that $\int_{\mathbf{R}^2} \left|\bar{F}_{R,S}(1+ia_1, 1+ia_2)\right| d(a_1,a_2) < \infty$. Write

$$\bar{F}_{R,S}(u,v) = 2^{1/4}u^{-3/2}e^{u/2}v^{-3/4}\left(\cosh\sqrt{2v}\right)^{-1/2}\left(\frac{\sqrt{2v}}{u} + \operatorname{arctanh}\sqrt{2v}\right)^{-1/2}.$$

Letting $u = 1 + ia_1$ and $v = 1 + ia_2$ with $a_1, a_2 \in \mathbf{R}$, then, as $\sqrt{a_1^2 + a_2^2} \to \infty$,

$$u^{-3/2} = O(|1 + a_1^2|^{-3/4}), \quad e^{u/2} = O(1), \quad v^{-3/4} = O(1),$$
$$\left(\cosh\sqrt{2v}\right)^{-1/2} = O(e^{-\operatorname{Re}\sqrt{2v}/2}) = O\left(e^{-\sqrt{|a_2|}/2}\right),$$
$$\left(\frac{\sqrt{2v}}{u} + \operatorname{arctanh}\sqrt{2v}\right)^{-1/2} = O\left\{\left(\frac{\sqrt{2v}}{u} + 1\right)^{-1/2}\right\} = O(1).$$

Hence $\left|\bar{F}_{R,S}(1 + ia_1, 1 + ia_2)\right| < C|1+a_1^2|^{-3/4}e^{-\sqrt{|a_2|}/2}$ for some constant $C > 0$, so that we deduce that $\int_{\mathbf{R}^2} \left|\bar{F}_{R,S}(1 + ia_1, 1 + ia_2)\right| d(a_1, a_2) < \infty$. Therefore, Proposition 2.6 implies:

Corollary 2.7 *The distribution function $F_{R,S}$ on $\mathbf{R}^2$ of (R, S) is continuous.*

2.2.2 A general proposition and the absolute continuity of (R, S)

We now proceed to the proof of the *absolute* continuity of (R, S) which again follows from a general criterion (Proposition 2.8).

Unlike probability density functions, (cumulative) distribution functions[7] on $\mathbf{R}^n$ are little common in the literature when $n \geq 2$. Under quite weak conditions we now state a general property which generalises an elementary property of one-dimensional distribution functions, namely that its continuous differentiability on some open set $D \subseteq \mathbf{R}$ of probability 1 implies its absolute continuity. The proposition is later applied to $F_{R,S}$.

Proposition 2.8 *Let F be a distribution function on $\mathbf{R}^n$ ($n = 1, 2, ...$) with associated probability measure $P := dF$. Suppose that there exist an open set $D \subseteq \mathbf{R}^n$ and a permutation $i_1, ..., i_n$ of $1, ..., n$, such these conditions hold:*

(i) $P(D) = 1$.

(ii) The n^{th} order partial derivative $\frac{d^n}{dx_{i_n} ... dx_{i_1}} F(x_1, ..., x_n)$ exists for all $(x_1, ..., x_n) \in D$ and defines a continuous function on D.

Then F is absolutely continuous and a density is given by the function defined as $\frac{d^n}{dx_{i_n} ... dx_{i_1}} F(x_1, ..., x_n)$ for $(x_1, ..., x_n) \in D$ and as 0 elsewhere.

Some remarks:

1. Surprisingly, we need not assume that the restriction $F|_D$ of F on D is a $C^n(D)$-function, i.e. is n times continuously differentiable. Of course, if

$F|_D \in C^n(D)$ then all m^{th} order partial derivatives exist and are continuous, implying (ii).

2. The density f may be discontinuous (e.g. tend to ∞) on part or all of the boundary of D.

3. As an *arbitrary* open set, D may be bounded or unbounded (e.g. $D = \mathbf{R}^n$), and may be connected or the union of disjoint open connected sets. The only impossible open set is $D = \emptyset$, since $P(D) = 1$.

PROOF. For technical simplicity we assume that $i_m = m$ for all $m = 1, ..., n$. The general case can be proved analogously. We have to prove that the function

$$f(x_1, ..., x_n) := \begin{cases} \frac{d^n}{dx_n...dx_1} F(x_1, ..., x_n) & \text{if } (x_1, ..., x_n) \in D, \\ 0 & \text{if } (x_1, ..., x_n) \notin D, \end{cases}$$

is a density of $P = dF$.

1. We first consider a "semi-open rectangle"

(2.13)
$$R := (x_1^1, x_1^2] \times ... \times (x_n^1, x_n^2] \subset D \quad \text{with} \quad -\infty < x_i^1 < x_i^2 < \infty \quad \forall i = 1, ..., n,$$

where, of course, the superscripts in x_i^1 and x_i^2 are indices, not powers. Write H_m for the m^{th} order (partial) differential operator $\frac{d^m}{dx_m...dx_1}$, where $m = 0, ..., n$. Note that $H_0F(x) = F(x)$ and $H_nF(x) = f(x)$ for all $x \in D$. The integral

$$I(R) := \int_R f(x)dx = \int_R H_nF(x)dx,$$

is well defined because f is continuous on the closure $\bar{R}$ of R. We show that $I(R) = P(R)$. By the theorem of Fubini,

$$I(R) = \int_{x_1^1}^{x_1^2} dx_1 \int_{x_2^1}^{x_2^2} dx_2 \cdots \int_{x_{n-1}^1}^{x_{n-1}^2} dx_{n-1} \int_{x_n^1}^{x_n^2} dx_n H_nF(x_1, ..., x_n),$$

and the idea is to apply the fundamental theorem of calculus n times, a formal proof being again by induction. First, we know by assumption that $H_nF(x_1, ..., x_n)$ is continuous with respect to $(x_1, ..., x_n) \in [x_1^1, x_1^2] \times ... \times [x_n^1, x_n^2]$. In particular, $H_nF(x_1, ..., x_n)$ is continuous with respect to $x_n \in [x_n^1, x_n^2]$, so that the inner integral becomes

$$\begin{aligned}
&\int_{x_n^1}^{x_n^2} dx_n H_n F(x_1, ..., x_n) \\
&= \int_{x_n^1}^{x_n^2} dx_n \frac{d}{dx_n} H_{n-1} F(x_1, ..., x_n) \\
&= \sum_{i=1}^{2} (-)^i H_{n-1} F(x_1, ..., x_{n-1}, x_n^i). \qquad (2.14)
\end{aligned}$$

Further, the continuity of the integrand $H_n F(x_1, ..., x_n)$ with respect to $(x_1, ..., x_n) \in [x_1^1, x_1^2] \times ... \times [x_n^1, x_n^2]$ implies the continuity of the integral (2.14) with respect to $(x_1, ..., x_{n-1}) \in [x_1^1, x_1^2] \times ... \times [x_{n-1}^1, x_{n-1}^2]$ (Forster, 1984, p. 82, Theorem 1). Now the next integral can be calculated analogously: By the continuity of $\int_{x_n^1}^{x_n^2} dx_n H_n F(x_1, ..., x_n)$ with respect to $x_{n-1} \in [x_{n-1}^1, x_{n-1}^2]$,

$$\begin{aligned}
&\int_{x_{n-1}^1}^{x_{n-1}^2} dx_{n-1} \int_{x_n^1}^{x_n^2} dx_n H_n F(x_1, ..., x_n) \\
&= \int_{x_{n-1}^1}^{x_{n-1}^2} dx_{n-1} \frac{d}{dx_{n-1}} \sum_{i=1}^{2} (-)^i H_{n-2} F(x_1, ..., x_{n-1}, x_n^i) \\
&= \sum_{i,j=1}^{2} (-)^{j+i} H_{n-2} F(x_1, ..., x_{n-2}, x_{n-1}^j, x_n^i), \qquad (2.15)
\end{aligned}$$

and again the continuity of the integrand $\int_{x_n^1}^{x_n^2} dx_n H_n F(x_1, ..., x_n)$ with respect to $(x_1, ..., x_{n-1}) \in [x_1^1, x_1^2] \times ... \times [x_{n-1}^1, x_{n-1}^2]$ implies the continuity of the integral (2.15) with respect to $(x_1, ..., x_{n-2}) \in [x_1^1, x_1^2] \times ... \times [x_{n-2}^1, x_{n-2}^2]$.

After n such steps one has calculated $I(R)$, viz.

$$I(R) = \sum_{i_1, ..., i_n = 1}^{2} (-)^{i_1 + ... + i_n} H_0 F(x_1^{i_1}, ..., , x_n^{i_n}) = \sum_{i_1, ..., i_n = 1}^{2} (-)^{i_1 + ... + i_n} F(x_1^{i_1}, ..., , x_n^{i_n}).$$

This coincides precisely with $P(R)$, as a straightforward generalisation of the case $n = 1$ where $P((x_1^1, x_1^2]) = F(x_1^2) - F(x_1^2)$.

2. To conclude, note first that $f(x) \geq 0$ for all $x \in D$: Indeed, if there were an $x \in D$ with $f(x) < 0$, then by the continuity of f on D there would exist a (small) semi-open rectangle R around x such that $f(y) < 0$ for all $y \in R$, implying the contradiction $P(R) = I(R) = \int_R f(x)dx < 0$.

Since f is a (measurable) non-negative function on D, a positive possibly unbounded (Borel-)measure on D can be defined by $\mu(B) := \int_B f(x)dx$ for Borel-sets $B \subseteq D$. By 1., μ coincides with P on the system $\mathcal{E}$ of all semi-open rectangles $R \subset D$. Since $\mathcal{E}$ is a generating system for the Borel-σ-algebra over D and since $\mathcal{E}$ is σ-finite and closed under finite intersections ($A, B \in \mathcal{E}$ implies $A \cap B \in \mathcal{E}$), the measures μ and P even coincide on all Borel sets in D by the uniqueness theorem for measure extensions (Billingsley,1986, p. 160, Theorem 10.3). So P is an absolutely continuous measure with density f. **QED**.

We are now in a position to deduce the absolute continuity of $F_{R,S}$.

Theorem 2.9 (R, S) *has an absolutely continuous distribution. It possesses a density* $f_{R,S}(r, s)$ *that is continuous on* $(-1/2, \infty) \times \mathbf{R}_+$ *and is 0 elsewhere.*

PROOF. The set $D := (-1/2, \infty) \times \mathbf{R}_+$ has the form prescribed in Proposition 2.8. By this proposition it is sufficient to show that for all $(r, s) \in D$ the derivative $\frac{d^2}{dsdr} F_{R,S}(r, s)$ exists and is continuous on D.

By the argumentwise inversion (2.11) of $\bar{F}_{R,S}(u, v)$ (as given by (2.12)),

$$\begin{aligned} F_{R,S}(r,s) &= \frac{1}{2\pi i}\int_{1+i\mathbf{R}} \frac{dv}{v} e^{sv} \\ &\times \frac{1}{2\pi i}\int_{1+i\mathbf{R}} \frac{du}{u} e^{(r+1/2)u} \left(\cosh\sqrt{2v} + \frac{u}{\sqrt{2v}}\sinh\sqrt{2v}\right)^{-1/2}. \end{aligned}$$

In this, the inner inversion is straightforward: it is the inversion, taken in $r + 1/2$, of a function of the form $au^{-1}(1 + ub)^{-1/2}$, with constants $a := \cosh^{-1/2}\sqrt{2v}$ and $b := \left(\tanh\sqrt{2v}\right)/\sqrt{2v}$. But $a(1 + ub)^{-1/2}$ is the Laplace transform of a rescaled $\chi^2(1)$ density, and hence $au^{-1}(1 + ub)^{-1/2}$ is the Laplace transform of a rescaled $\chi^2(1)$ distribution function. We deduce that the inner inverse equals

$$\begin{aligned} \int_0^{r+1/2} \frac{a}{\sqrt{\pi r'}} e^{-r'/b} b^{-1/2} dr' &= \left(\frac{1}{\sqrt{2v}}\sinh\sqrt{2v}\right)^{-1/2} \\ &\times \int_0^{r+1/2} \frac{1}{\sqrt{\pi r'}} \exp\left(\frac{-r'\sqrt{2v}}{\tanh\sqrt{2v}}\right) dr'. \end{aligned}$$

So

$$F_{R,S}(r,s) = \frac{1}{2\pi i}\int_{1+i\mathbf{R}} \frac{dv}{v} e^{sv} \left(\frac{1}{\sqrt{2v}}\sinh\sqrt{2v}\right)^{-1/2}$$
$$\times \int_0^{r+1/2} \frac{1}{\sqrt{\pi r'}} \exp\left(\frac{-r'\sqrt{2v}}{\tanh\sqrt{2v}}\right) dr'.$$

In this, the integrand of the outer integral is (partially) differentiable with respect to $r > -1/2$, with derivative given by:
(2.16)

$$g(v,r,s) = \frac{1}{v}e^{sv}\left(\frac{1}{\sqrt{2v}}\sinh\sqrt{2v}\right)^{-1/2} \frac{1}{\sqrt{\pi(r+1/2)}} \exp\left(\frac{-(r+1/2)\sqrt{2v}}{\tanh\sqrt{2v}}\right).$$

For fixed s, the function $v \mapsto g(v,r,s)$ is (with respect to r) locally uniformly bounded by a (with respect to $v \in 1+i\mathbf{R}$) integrable function[8], so that the integral $F_{R,S}(r,s)$ is (partially) differentiable with respect to $r > -1/2$ and

$$\frac{d}{dr}F_{R,S}(r,s) = \frac{1}{2\pi i}\int_{1+i\mathbf{R}} g(v,r,s)dv, \quad (r,s) \in D. \tag{2.17}$$

This "differenciability under the integral sign" is a consequence of the dominated convergence theorem; see for instance Jones (1993, p. 154). We now use this argument a second time: the integrand $g(v,r,s)$ is (partially) differentiable with respect to each $s > 0$, with derivative $\frac{d}{ds}g(v,r,s) = vg(v,r,s)$. For fixed r, the function $v \mapsto vg(v,r,s)$ is (with respect to s) locally uniformly bounded by a (with respect to $v \in 1+i\mathbf{R}$) integrable function[8], so that $\frac{d}{dr}F_{R,S}(r,s)$ is (partially) differentiable with respect to each $s > 0$ and

$$\frac{d}{dsdr}F_{R,S}(r,s) = \frac{1}{2\pi i}\int_{1+i\mathbf{R}} vg(v,r,s)dv, \quad (r,s) \in D. \tag{2.18}$$

Finally, the integrand $vg(v,r,s)$ is continuous in the pair $(r,s) \in D$, and the function $v \mapsto vg(v,r,s)$ is (with respect to (r,s)) locally uniformly bounded by a (with respect to $v \in 1+i\mathbf{R}$) integrable function[8], so that the integral $\frac{d}{dsdr}F_{R,S}(r,s)$ is continuous in $(r,s) \in D$; this argument follows immediately from the dominated convergence theorem. **QED**.

[8] A function $h(v,t)$, where $v \in 1+i\mathbf{R}$ and t belongs to some metric space $\mathcal{T}$, is "locally uniformly bounded by an integrable function" if each $t_0 \in \mathcal{T}$ possesses a neighbourhood $A \ni t_0$ and there exists a positive function $\bar{h}(v)$ not depending on t, such that $\bar{h}(v)$ is integrable (over $v \in 1+i\mathbf{R}$) and satisfies $|h(v,t)| \leq \bar{h}(v)$ $\forall t \in A$ and $\forall v \in 1+i\mathbf{R}$.

Corollary 2.10 *The distribution functions F_τ and F_κ are continuous.*

PROOF. Let $z \in \mathbf{R}$. It is to be shown that $P(\tau = z) = 0$ and $P(\kappa = z) = 0$. We have $P(\tau = z) = P((R, S) \in B_z)$ where B_z is the Borel set $B_z := \{(r, s) \in (-1/2, \infty) \times \mathbf{R}_+ | r = z\sqrt{s}\}$. Since B_z has Lebesgue-measure $\lambda^2(B_z) = 0$, the absolute continuity of (R, S) implies that $P((R, S) \in B_z) = 0$. The argument for $P(\kappa = z) = 0$ is analogous. **QED**.

2.3 The normalised coefficient estimator

We first analyse the limiting variable $\kappa = R/S$ (cf. Corollary 2.2 above) since the derivations are slightly easier than for $\tau = R/\sqrt{S}$. Our focus is on the (cumulative) distribution function $F_\kappa(z) := P(\kappa \leq z)$ where $z \in \mathbf{R}$ for which we derive closed expressions (cf. Dietrich 2002a). (The density $f_\kappa(z)$ is discussed in Section 2.5.) We distinguish between the cases $z = 0$, $z < 0$ and $z > 0$. The case $z = 0$ is known and trivial (cf. Section 2.3.1). For $z < 0$, Section 3.3.2 recapitulates Abadir's (1993) formula for $F_\kappa(z)$, carefully stating the properties used such as the continuity of F_κ (Corollary 2.10) which Abadir implicitly assumes. We also prove a new related formula for $F_\kappa(z)$ which will later be seen to have some numerical advantages, such as in particular the existence of a comfortable truncation criterion for the inner series. For $z > 1/2$, Section 3.3.3 derives two formulae which are the first such expressions for positive z; the validity of the latter formulae when $0 < z \leq 1/2$ can be conjectured, but we are unable to give a proof. While the formulae of Sections 3.3.2 and 3.3.3 each contain two infinite series and one finite sum, Section 3.3.4 derives an expression with only one infinite series, but two finite sums, valid for $z < 0$. All derived formulae (except when $z = 0$) contain the parabolic cylinder function $D_p(\zeta)$ (see Appendix A).

2.3.1 Case of $z = 0$

We have $F_\kappa(0) = P(R/S \leq 0) = P(R \leq 0)$. Since R has $\chi^2(1)/2 - 1/2$ distribution, $F_\kappa(0)$ is the probability that a $\chi^2(1)/2 - 1/2$ variable is at most 0, i.e. that a $\chi^2(1)$ variable is at most 1:

$$F_\kappa(0) = \frac{1}{\sqrt{2\pi}} \int_0^1 x^{-1/2} e^{-x/2} dx = \frac{2}{\sqrt{\pi}} \int_0^{2^{-1/2}} e^{-x^2} dx = \operatorname{erf}(2^{-1/2}) \\ \approx 0.682689492137.$$

2.3.2 Case of $z \neq 0$: applying Gurland's theorem

Let $z \neq 0$. Abadir (1993) uses Gurland's (1948, p. 229-230, Theorem 1) general tool for the derivation of the distribution of a ratio. This tool applies as follows to $\kappa = R/S$. By noting that $F_\kappa(z) = P(\kappa \leq z) = P(Q \leq 0) = F_Q(0)$ where $Q := R - zS$, Gurland proves an inversion formula which (after a change of variable) can be written as:

$$\frac{1}{2}\left[F_\kappa(z) + \lim_{t \uparrow z} F_\kappa(t)\right] = \frac{1}{2} + \frac{1}{2\pi i} \lim_{r\downarrow 0, R\uparrow\infty} \left(\int_{-iR}^{-ir} + \int_{ir}^{iR}\right) \frac{1}{v} \exp(-vQ) dv,$$

where the Laplace transform of Q follows from that of (R, S) via $\exp(-vQ) = \exp(-vR + vzS)$. Now, the left hand side is $F_\kappa(z)$ by the continuity of F_κ (Corollary 2.10). So (after substituting $-2v/z$ for v), we have

$$\begin{aligned} F_\kappa(z) &= \frac{1}{2} + \operatorname{sgn}(-z)\frac{1}{2\pi i} \\ &\times \lim_{r\downarrow 0} \left(\int_{-i\infty}^{-ir} + \int_{ir}^{i\infty}\right) \frac{1}{v} e^{-v/z} \left(\cosh\sqrt{4v} - \frac{\sqrt{v}}{z}\sinh\sqrt{4v}\right)^{-1/2} dv. \end{aligned}$$

The power series of cosh and sinh show that the integrand is holomorphic in a neighbourhood of $v = 0$ except in $v = 0$ where it has a simple pole with residual 1. Hence $(2\pi i)^{-1}$ times its integral along the counter-clockwise *semi-circle* $re^{i\theta}, \theta \in [-\pi/2, \pi/2]$ tends to 1/2 times its residue in $v = 0$, i.e. to 1/2, as $r \downarrow 0$ (Priestley, 1990, p. 115). So

(2.19) $$F_\kappa(z) = \begin{cases} G(z) & \text{if } z < 0 \\ 1 - G(z) & \text{if } z > 0 \end{cases}$$

where

(2.20) $$G(z) := \frac{1}{2\pi i} \int_{P_\varepsilon} \frac{1}{v} e^{-v/z} \left(\cosh\sqrt{4v} - \frac{\sqrt{v}}{z}\sinh\sqrt{4v}\right)^{-1/2} dv$$

and the path P_ε is the union of the straight line $(-i\infty, -i\varepsilon)$, the counter-clockwise semi-circle $\theta \mapsto \varepsilon e^{i\theta}$, $\theta \in [-\pi/2, \pi/2]$, and the straight line $(i\varepsilon, i\infty)$.

The parameter $\varepsilon > 0$ has to be chosen small enough so that the integrand has no singularity between the imaginary axis and P_ε, nor on P_ε. The complex

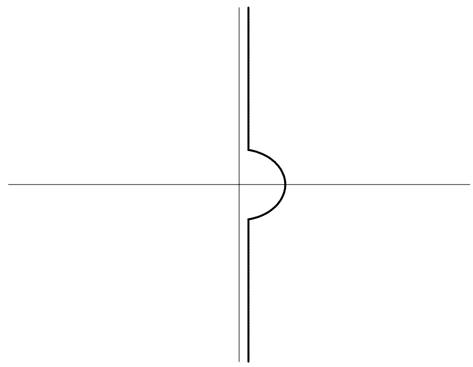

Figure 2.1: The path P_ε

square root $\sqrt{\zeta}$ is interpreted as having the argument $\theta/2$ where $\theta := \arg(\zeta) \in (-\pi, \pi]$.

In (2.20), despite the square roots, the expression in brackets is an entire function of $v \in \mathbf{C}$ which is real on $v \in \mathbf{R}$ and takes the value 1 at $v = 0$. This can be seen from the power series of cosh and sinh . The entire function is raised to the power $-1/2$, so that the integrand in $G(z)$ becomes a multi-function of v whose branch points are the nulls (if existent) of the entire function. The relevant branch is determined by having positive value (at least) in a real neighbourhood of $v = 0$. This is because $\exp(-vQ)$ – if existent – is positive for real v. Besides branch points (if existent), the only other singularity of the integrand is the simple pole $v = 0$.

2.3.3 Case of $z < 0$: Abadir's and a related formula for $F_\kappa(z)$

It is helpful to be quite explicit and precise about the steps of the following derivation which is largely identical for Abadir's and our new formula for $F_\kappa(z)$ where $z < 0$. This will help understanding the additional difficulties encountered in the next section where $z > 0$.

The starting point of the expansions of both this section (where $z < 0$) and the next section (where $z > 0$) is Abadir's transformation:

$$\cosh\sqrt{4v} - \frac{\sqrt{v}}{z}\sinh\sqrt{4v} = \frac{1}{2}\left\{e^{2\sqrt{v}}\left(1-\frac{\sqrt{v}}{z}\right) + e^{-2\sqrt{v}}\left(1+\frac{\sqrt{v}}{z}\right)\right\}$$

$$(2.21) \qquad = \frac{1}{2}e^{2\sqrt{v}}\left(1-\frac{\sqrt{v}}{z}\right)\left(1+e^{-4\sqrt{v}}\frac{1+\sqrt{v}/z}{1-\sqrt{v}/z}\right),$$

Now assume that $z < 0$. Then the function (2.21) has no nulls: Indeed, since $\mathrm{Re}\sqrt{v} \geq 0$, the first bracket is obviously non-zero, and the second bracket is non-zero because

$$(2.22) \qquad \left|e^{-4\sqrt{v}}\frac{1+\sqrt{v}/z}{1-\sqrt{v}/z}\right| < 1$$

since $|1+\sqrt{v}/z| \leq |1-\sqrt{v}/z|$. Hence the integrand in (2.20) has no singularities other than the pole $v = 0$, and no care has to be taken in the choice of P_ε. By (2.22), Abadir (1993, p. 1060, (2.6)) can expand:

$$\left(\cosh\sqrt{4v} - \frac{\sqrt{v}}{z}\sinh\sqrt{4v}\right)^{-1/2} = \sqrt{2}e^{-\sqrt{v}}\left(1-\frac{\sqrt{v}}{z}\right)^{-1/2}$$

$$(2.23) \qquad \times\sum_{j=0}^{\infty}\binom{-1/2}{j}e^{-4j\sqrt{v}}\left(\frac{1+\sqrt{v}/z}{1-\sqrt{v}/z}\right)^{j}.$$

In this, Abadir (1993, bottom of p. 1060) further writes

$$(2.24) \quad \left(\frac{1+\sqrt{v}/z}{1-\sqrt{v}/z}\right)^{j} = \left(\frac{2}{1-\sqrt{v}/z}-1\right)^{j} = \sum_{l=0}^{j}\binom{j}{l}(-)^{j+l}2^{l}\left(1-\frac{\sqrt{v}}{z}\right)^{-l}.$$

Using the dominated convergence theorem, (2.20) now becomes

$$(2.25) \qquad G(z) = \sqrt{2}\sum_{j=0}^{\infty}\binom{j-1/2}{j}\sum_{l=0}^{j}\binom{j}{l}(-2)^{l}I_{jl}(z),$$

with termwise integral

$$(2.26) \qquad I_{jl}(z) := \frac{1}{2\pi i}\int_{P_\varepsilon}\frac{1}{v}e^{-v/z-(4j+1)\sqrt{v}}\left(1-\frac{\sqrt{v}}{z}\right)^{-l-1/2}dv.$$

In order to be able to compute this Laplace inverse, Abadir expands

$$(2.27) \qquad \frac{1}{v} = \frac{-1}{z\sqrt{v}}\left\{\left(1-\frac{\sqrt{v}}{z}\right)-1\right\}^{-1} = \frac{-1}{z\sqrt{v}}\sum_{k=0}^{\infty}\left(1-\frac{\sqrt{v}}{z}\right)^{-k-1},$$

which is possible because $|1-\sqrt{v}/z| > 1$ for $v \in P_\varepsilon$. Applying again the dominated convergence theorem and then substituting $\sqrt{w} = 1-\sqrt{v}/z$ yields

$$\begin{aligned} I_{jl}(z) &= \sum_{k=0}^{\infty} \frac{1}{2\pi i} \int_{P_\varepsilon} \frac{-1}{z\sqrt{v}} e^{-v/z-(4j+1)\sqrt{v}} \left(1-\frac{\sqrt{v}}{z}\right)^{-l-k-3/2} dv \\ &= e^{-z(4j+2)} \sum_{k=0}^{\infty} \frac{1}{2\pi i} \int_{P'_\varepsilon} e^{-zw+z(4j+3)\sqrt{w}} w^{-l/2-k/2-5/4} dw. \end{aligned}$$

Since the new path P'_ε like P_ε goes from $-i\infty$ to $i\infty$ by passing to the right of the singularity 0, the last integral is recognized as a Laplace inverse which can be expressed in terms of the parabolic cylinder function, cf. Prudnikov and Brychkov and Marichev, 1992, p. 52, 10. After substituting the resulting expression of $I_{jk}(z)$ into $G(z)$, and remembering that $F_\kappa(z) = G(z)$ for $z < 0$, Abadir's formula for $F_\kappa(z)$ is obtained as given by the first expression in Theorem 2.11 below.

Given that the author is unable to give a simple upper bound for the error from truncating the series in k of Abadir's expression, we now derive a new formula (second expression in Theorem 2.11) by choosing slightly different expansions in $l = 0, ..., j$ and $k = 0, ..., \infty$: Instead of (2.24) we now write

$$\left(\frac{1+\sqrt{v}/z}{1-\sqrt{v}/z}\right)^j = \left(1+\frac{2\sqrt{v}/z}{1-\sqrt{v}/z}\right)^j = \sum_{l=0}^{j} \binom{j}{l} 2^l \left(\frac{\sqrt{v}/z}{1-\sqrt{v}/z}\right)^l,$$

in which we use the fact that $\frac{\sqrt{v}/z}{1-\sqrt{v}/z} = \frac{1}{1-\sqrt{v}/z} - 1$ to further expand:

$$\left(\frac{\sqrt{v}/z}{1-\sqrt{v}/z}\right)^l = (-)^{l+1} \frac{\sqrt{v}/z}{1-\sqrt{v}/z} \sum_{k=0}^{\infty} \binom{l-1}{k} (-)^k \left(1-\frac{\sqrt{v}}{z}\right)^{-k}.$$

Hence we have

$$\left(\frac{1+\sqrt{v}/z}{1-\sqrt{v}/z}\right)^j = \frac{-\sqrt{v}}{z} \sum_{k=0}^{\infty} c(j,k) \left(1-\frac{\sqrt{v}}{z}\right)^{-k-1}, \tag{2.28}$$

where the coefficient $c(j,k)$ satisfies

(2.29)

$$c(j,k) := (-)^k \sum_{l=0}^{j} \binom{j}{l} \binom{l-1}{k} (-2)^l = 1 + (-)^k \sum_{l=k+1}^{j} \binom{j}{l} \binom{l-1}{k} (-2)^l$$

since $\binom{l-1}{k}$ is 0 if $1 \leq l \leq k$ and is $(-)^k$ if $l = 0$. Note that if $k \geq j$ the last sum is empty and $c(j,k) = 1$. Some nice representations of $c(j,k)$ are proven soon (Proposition 2.12)

The new expression for $F_\kappa(z)$ follows by combining (2.28) with (2.23), (2.20) and (2.19), and then applying the dominated convergence theorem and again expressing the termwise integral in terms of the parabolic cylinder function as in Prudnikov and Brychkov and Marichev (1992, p. 52, 10):

Theorem 2.11 *Let $z < 0$ and put $y := \sqrt{2|z|}$. The limiting distribution function of κ satisfies $F_\kappa(z) = \sum_{j=0}^{\infty} F_j(z)$ where the summand $F_j(z)$ has the two expressions:*

$$\begin{aligned} F_j(z) &= 2\sqrt{\frac{y}{\pi}} \binom{j-1/2}{j} e^{-y^2(j^2-j/2-7/16)} \sum_{k=0}^{\infty} y^k \sum_{l=0}^{j} \binom{j}{l} (-2y)^l \\ &\qquad\qquad\qquad\qquad\qquad\qquad \times D_{-l-k-3/2}\left(y(2j+3/2)\right) \\ &= 2\sqrt{\frac{y}{\pi}} \binom{-1/2}{j} e^{-y^2(j^2-j/2-7/16)} \sum_{k=0}^{\infty} c(j,k) y^k D_{-k-3/2}\left(y(2j+3/2)\right). \end{aligned}$$

Here $c(j,k)$ is given by (2.29) or Proposition 2.12 below and equals 1 if $k \geq j$.

See Appendix A for the parabolic cylinder function $D_p(\zeta)$. The first expression differs from Abadir's (1993, p. 1062, (2.8)) expression only in that he considers $\kappa/\sqrt{2}$ instead of κ (resulting in a different definition of y), and in that we have interchanged the summations in l and k, and in that Abadir expresses $j^2 - j/2 - 7/16$ as $(2j+1/2)^2/2 - (2j+3/2)^2/4$ which allows (in both formulae) to identify the hypergeometric function $K(p,\zeta) := e^{\zeta^2/4} D_p(\zeta)$.

As an advantage of the second expression, the coefficient $c(j,k)$ can be expressed in terms of special functions where the expression (2.32)-(2.33) below contains desirable numerical properties (cf. Section 4.4):

Proposition 2.12 *If $j \leq k$ then $c(j,k) = 1$. If $j > k$ then $c(j,k)$ can be* *expressed in two ways in terms of terminating hypergeometric series:*

$$c(j,k) = 1 - 2^{k+1}\frac{j-k}{k+1}\binom{j}{k}\,{}_2F_1(k+1-j, k+1; k+2; 2) \tag{2.30}$$

$$= 1 - 2^{k+1}\frac{j!}{k!}\sum_{l=0}^{j-k-1}\frac{(-2)^l}{l!(j-k-1-l)!(l+k+1)}, \tag{2.31}$$

$$c(j,k) = (-)^{j-k}\binom{j}{k}\,{}_2F_1(-k, j-k; j-k+1; -1) \tag{2.32}$$

$$= (-)^{j-k}\frac{j!}{(j-k-1)!}\sum_{l=0}^{k}\frac{1}{l!(k-l)!(l+j-k)}, \tag{2.33}$$

and in two ways in terms of the incomplete beta function:

$$c(j,k) = 1-(j-k)\binom{j}{k}\beta_2(k+1, j-k) = (j-k)\binom{j}{k}\beta_{-1}(j-k, k+1). \tag{2.34}$$

Note that if $p, q = 1, 2, ...$ then $\beta_\zeta(p,q)$ is an entire[9] functions of $\zeta \in \mathbf{C}$ whose value is uniquely given by the integral $\int_0^\zeta t^{p-1}(1-t)^{q-1}\,dt$.

Proof of Proposition 2.12. Let $j > k$. One easily derives the equality of the right hand side of (2.30) to (2.31), and the equality of the right hand side of (2.32) to (2.33). Moreover, (2.31) can be transformed into (2.29) by substituting $l-k-1$ for l. Further, the expression with ${}_2F_1(.,.;.;2)$ equals the expression with $\beta_2(p,q)$, and the expression with ${}_2F_1(.,.;.;-1)$ equals the expression with $\beta_{-1}(p,q)$, see Erdélyi (1953), vol. 1, p. 87.

The proof is completed by showing that the expression with $\beta_2(.,.)$ equals that with $\beta_{-1}(.,.)$. First, we decompose:

$$\beta_2(k+1, j-k) = \int_0^2 t^k(1-t)^{j-k-1}dt = \beta(k+1, j-k) + \int_1^2 t^k(1-t)^{j-k-1}dt.$$

Using the relation $\beta(p,q) = \Gamma(p)\Gamma(q)/\Gamma(p+q)$ and substituting $t = 1-s$ in the last integral,

$$\beta_2(k+1, j-k) = \frac{k!(j-k-1)!}{j!} - \beta_{-1}(j-k, k+1). \quad \textbf{QED}.$$

[9]That means, these functions are holomorphic on the entire plane $\zeta \in \mathbf{C}$. In particular, they are single-valued and hence uniquely defined.

For numerical purposes, let us consider the magnitude of $c(j,k)$. The second beta expression for $c(j,k)$ allows to derive this bound:

Corollary 2.13 *If $j > k$, then*

$$0 < (-)^{j-k} c(j,k) < 2^k \binom{j}{k}.$$

Proof. Since

$$\begin{aligned} c(j,k) &= (j-k)\binom{j}{k} \int_0^{-1} t^{j-k-1}(1-t)^k dt \\ &= (-)^{j-k}(j-k)\binom{j}{k} \int_0^{1} t^{j-k-1}(1+t)^k dt, \end{aligned}$$

we have

$$0 < (-)^{j-k} c(j,k) < (j-k)\binom{j}{k} 2^k \int_0^1 t^{j-k-1} dt = 2^k \binom{j}{k}. \textbf{ QED}.$$

2.3.4 Case of $z > 0$: two formulae for $F_\kappa(z)$

Now assume that $z > 0$. In order to derive formulae for $F_\kappa(z)$ we again start with the series expansion (2.23). However, this expansion may not converge since for $z > 0$ the inequality (2.22) may not hold for all v on the integration path P_ε. In Lemma 2.14 we prove that, for suitable ε, the expansion works provided that $z > 1/2$. Although this expansion of the integrand in the integral (2.20) for $G(z)$ diverges on part of P_ε when $0 < z \leq 1/2$, numerical tests indicate that (a) after applying the integration to the individual summands of the integrand expansion the series now converges *for all* $z > 0$, and that (b) the limit is indeed $G(z)$ even when $z \leq 1/2$. However, the author is unable to prove (a) and (b), and hence the correctness when $0 < z \leq 1/2$ of this section's formulae for $F_\kappa(z)$ is left as an unproven conjecture. Note that if (a) was true then (b) would be no surprise since the limit in (a), say $\bar{G}(z)$, is likely to define a holomorphic function in a neighbourhood of each $z \in \mathbf{R}_+$, just as $G(z)$ does by (2.20); if so, then the identity $\bar{G}(z) = G(z)$ which holds for $z \in (1/2, \infty)$ even holds for $z \in \mathbf{R}_+$ by the identity theorem of complex analysis (Priestley, 1990, p. 73).

Lemma 2.14 *Assume that $z > 1/2$. Then in* (2.20) *the parameter ε can be chosen such that the path P_ε satisfies the inequality* (2.22).

PROOF. We have to prove that there is an $\varepsilon := \varepsilon(z) > 0$ such that

(i) the integrand of (2.20) has no singularity on $v \in \{\zeta | \operatorname{Re}\zeta \geq 0 \text{ and } |\zeta| \leq \varepsilon\}$, and

(ii) the inequality (2.22) holds for $v \in P_\varepsilon$.

These conditions hold if

(iii) the inequality (2.22) holds for $v \in P_\varepsilon \cup \{\zeta | \operatorname{Re}\zeta \geq 0 \text{ and } |\zeta| \leq \varepsilon\}$.

Indeed, (iii) immediately implies (ii). Regarding (i), since the singularities of (2.20) (except $v = 0$) are the nulls of (2.21), we have to show that no $v \in \{\zeta | \operatorname{Re}\zeta \geq 0 \text{ and } |\zeta| \leq \varepsilon\}$ is a null of (2.21). This is true because (iii) implies that

$$1 - \frac{\sqrt{v}}{z} \neq 0 \quad \text{and} \quad 1 + e^{-4\sqrt{v}} \frac{1 + \sqrt{v}/z}{1 - \sqrt{v}/z} \neq 0.$$

So we have to prove the existence of an $\varepsilon := \varepsilon(z) > 0$ satisfying (iii). Since v belongs to $P_\varepsilon \cup \{\zeta | \operatorname{Re}\zeta \geq 0 \text{ and } |\zeta| \leq \varepsilon\}$ if and only if $w := \sqrt{v}$ belongs to $\{\zeta | \arg\zeta = \pm\pi/4\} \cup \{\zeta | -\pi/4 \leq \arg\zeta \leq \pi/4 \text{ and } |\zeta| \leq \sqrt{\varepsilon}\}$, we may equivalently prove the existence of a $\delta > 0$ such that:

(iv) $\left| e^{-4w} \frac{1+w/z}{1-w/z} \right| < 1$ for all $w \in \{\zeta | \arg\zeta = \pm\pi/4\} \cup \{\zeta | -\pi/4 \leq \arg\zeta \leq \pi/4$ and $|\zeta| \leq \delta\}$.

By first order Taylor expansion, as $w \to 0$,

$$\begin{aligned} e^{-4w} \frac{1 + w/z}{1 - w/z} &= (1 - 4w + O(w^2)) \left(1 + \frac{w}{z}\right) \left(1 + \frac{w}{z} + O(w^2)\right) \\ &= 1 - \left(4 - \frac{2}{z}\right) w + O(w^2). \end{aligned}$$

In this, since $z > 1/2$ we have $4 - 2/z > 0$. Hence there exists a $\delta > 0$ such that the inequality in (iv) holds at least for $w \in \{\zeta | -\pi/4 \leq \arg\zeta \leq \pi/4$ and $|\zeta| \leq \delta\}$.

We now show that the inequality also holds when $w \in \{\zeta | \arg\zeta = \pm\pi/4\}$. Such a w can be written as $t(1 \pm i)$ for some real $t > 0$. Without loss of generality we assume that $\arg w = +\pi/4$, i.e. $w = t(1 + i)$: indeed, if the inequality holds for w it also holds for the complex conjugate $\overline{w} = t(1-i)$, because

$$\left| e^{-4\overline{w}} \frac{1+\overline{w}/z}{1-\overline{w}/z} \right| = \left| \overline{e^{-4w} \frac{1+w/z}{1-w/z}} \right| = \left| e^{-4w} \frac{1+w/z}{1-w/z} \right|.$$

Putting $w = t(1+i) = zs(1+i)$ (with $s := t/z$), we calculate

$$\left| e^{-4w} \frac{1+w/z}{1-w/z} \right|^2 = e^{-8zs\,\mathrm{Re}(1+i)} \frac{(1+s)^2+s^2}{(1-s)^2+(-s)^2} = e^{-8zs} \frac{1+2s+2s^2}{1-2s+2s^2}.$$

To show that this is smaller than 1 for all $s > 0$, we may put $z = 1/2$; indeed, since the expression is decreasing in z, if the inequality holds for $z = 1/2$ then it does so too for every $z > 1/2$. Hence it is sufficient to prove that

$$e^{-4s} \frac{1+2s+2s^2}{1-2s+2s^2} < 1 \quad \text{for all } s > 0. \tag{2.35}$$

We first show this in in a neighbourhood of the origin $s = 0$. By a 3$^{\text{rd}}$ order Taylor expansion, for some $\zeta \in (-4s, 0)$,

$$e^{-4s} = \sum_{n=0}^{3} (-)^n \frac{(4s)^n}{n!} + \frac{(4s)^4}{4!} e^{-\zeta} < \sum_{n=0}^{4} (-)^n \frac{(4s)^n}{n!}.$$

After substituting this bound in (2.35), and then on each side multiplying by and thereafter subtracting $1 - 2s + 2s^2$, we have to show that

$$\left\{ \sum_{n=0}^{4} (-)^n \frac{(4s)^n}{n!} \right\} (1+2s+2s^2) - (1-2s+2s^2) < 0.$$

By expanding the product and simplifying, the terms in s^0, s^1 and s^2 cancel out, so that, after dividing by $8s^3/3$, we obtain

$$8s^3 + 2s - 1 < 0,$$

which can be solved analytically to give

$$s < s_0 := \sqrt[3]{\sqrt{12^{-3} + 16^{-2}} + 16^{-1}} - \sqrt[3]{\sqrt{12^{-3} + 16^{-2}} - 16^{-1}} \approx 0.341164.$$

For the case that $s \geq s_0$ we need a different approach to show (2.35). Since the denominator $1 - 2s + 2s^2$ of (2.35) is minimal in $s = 1/2$ where it takes the value $2(1/2)^2 - 2/2 + 1 = 1/2$, it is sufficient to show that

$$2e^{-4s}(1+2s+2s^2) < 1 \quad \text{for all } s \geq s_0.$$

This inequality holds for $s = s_0$ since $2e^{-4s_0}(1 + 2s_0 + 2s_0^2) \approx 0.978503$. Hence it is sufficient to show that $2e^{-4s}(1+2s+2s^2)$ is a decreasing function of $s > 0$, which follows from

$$\frac{d}{ds}\ln\left\{2e^{-4s}(1 + 2s + 2s^2)\right\} = -4 + \frac{2 + 4s}{1 + 2s + 2s^2} < -4 + \frac{2 + 4s}{1 + 2s} < 0. \ \textbf{QED}.$$

By assuming that $z > 1/2$ we can now proceed with the derivation of formulae for $F_\kappa(z)$. By Lemma 2.14 we can make the same expansion in j as for $z < 0$, which yields the expression (2.25) for $G(z)$ with the remaining integral given by:

$$I_{jl}(z) = \frac{1}{2\pi i}\int_{P_\varepsilon} \frac{1}{v} e^{-v/z-(4j+1)\sqrt{v}} \left(1 - \frac{\sqrt{v}}{z}\right)^{-l-1/2} dv.$$

When $z < 0$, this could be calculated by writing v^{-1} as $v^{-1/2}$ times a descending power series in $1-\sqrt{v}/z$, cf. (2.27). However, if $z > 0$ then neither a descending nor an ascending power series in $1 - \sqrt{v}/z$ is possible, because $|1 - \sqrt{v}/z|$ can become both smaller than 1 (for v on the circular part of P_ε) and greater than 1 (for large v). We will tackle this problem by transforming the path.

Note first that P_ε goes from $-i\infty$ to $i\infty$ by passing between the two branch points $v = 0$ and $v = z^2$. In order to turn the branch point $v = 0$ into a pole of order 1, we substitute $\sqrt{v} = w$; after deforming the path,

$$I_{jl}(z) = \frac{1}{2\pi i}\int_{\infty}^{(z-)} \frac{2}{w} e^{-w^2/z-(4j+1)w} \left(1 - \frac{w}{z}\right)^{-l-1/2} dw, \tag{2.36}$$

where as shown in Figure 2.2 the notation "$\int_\infty^{(a+)}$" respectively "$\int_\infty^{(a-)}$" stands for integration along a path going from ∞ to ∞ by encircling the point $a \in \mathbf{C}$ (and no other point b which is a singularity to the left of a, i.e. $\operatorname{Re} b < \operatorname{Re} a$) in the counter-clockwise respectively clockwise sense and such that $|\arg(a-w)| < \pi$ for w on the path.

In the new integrand, 0 is now a pole with residue 2. So, by the residue theorem,

$$I_{jl}(z) = 2 + \frac{1}{2\pi i}\int_{\infty}^{(0-)} \frac{2}{w} e^{-w^2/z-(4j+1)w} \left(1 - \frac{w}{z}\right)^{-l-1/2} dw. \tag{2.37}$$

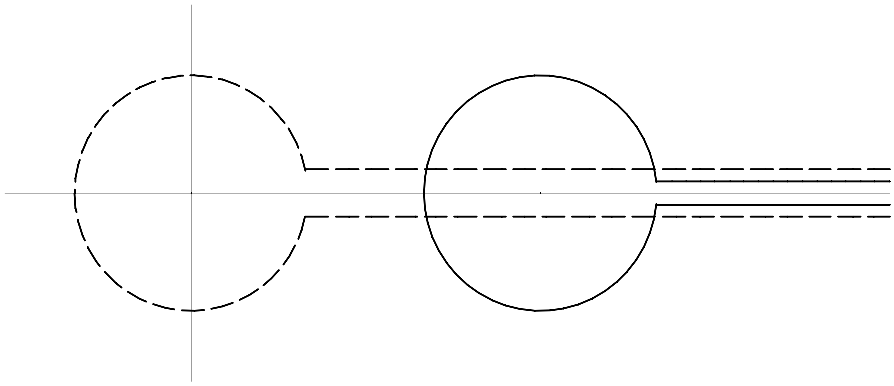

Figure 2.2: The paths of the integrals in (2.36) (full line) and (2.37) (dashed line).

In this integral, the path (Figure 2.2) can be chosen such that $|1 - w/z| > 1$, which enables an expansion in descending powers of $1 - w/z$:

$$\frac{1}{w} = \frac{-1}{z}\left\{\left(1 - \frac{w}{z}\right) - 1\right\}^{-1} = \frac{-1}{z}\sum_{k=0}^{\infty}\left(1 - \frac{w}{z}\right)^{-k-1}. \tag{2.38}$$

So, by the dominated convergence theorem,

$$I_{jl}(z) = 2 + \frac{2}{z}\sum_{k=0}^{\infty}\frac{1}{2\pi i}\int_{\infty}^{(z+)} e^{-w^2/z-(4j+1)w}\left(1 - \frac{w}{z}\right)^{-l-k-3/2} dw.$$

Notice that the integral is now in the counter-clockwise sense (which changes the sign of the integral) and that the integral encircles z instead of 0 since 0 is no longer a singularity. Finally, substituting $-w$ for $1 - w/z$,

$$I_{jl}(z) = 2 + 2e^{-z(4j+2)}\sum_{k=0}^{\infty}\frac{1}{2\pi i}\int_{\infty}^{(0+)} e^{-zw^2-z(4j+3)w}(-w)^{-l-k-3/2}dw.$$

By Gradshteyn and Ryzhik (1994), p. 1092, 9.242, 1., the last integral can be expressed in terms of the parabolic cylinder function:

$$I_{jl}(z) = 2 - 2e^{y^2(j^2-j/2-7/16)}\sum_{k=0}^{\infty} y^{l+k+1/2}\frac{D_{l+k+1/2}\left(y(2j+3/2)\right)}{\Gamma(l+k+3/2)},$$

where $y := \sqrt{2|z|} = \sqrt{2z}$ as in Theorem 2.11. Now we obtain:

$$\begin{aligned} G(z) &= \sqrt{2}\sum_{j=0}^{\infty}\binom{j-1/2}{j}\sum_{l=0}^{j}\binom{j}{l}(-2)^l I_{jk}(z) \\ &= 2-\sqrt{8y}\sum_{j=0}^{\infty}\binom{j-1/2}{j}e^{y^2(j^2-j/2-7/16)}\sum_{l=0}^{j}\binom{j}{l}(-2y)^l \\ &\qquad\times\sum_{k=0}^{\infty}y^k\frac{D_{l+k+1/2}\left(y(2j+3/2)\right)}{\Gamma(l+k+3/2)}, \end{aligned}$$

because

$$\sum_{j=0}^{\infty}\binom{j-1/2}{j}\sum_{l=0}^{j}\binom{j}{l}(-2)^l = \sum_{j=0}^{\infty}\binom{j-1/2}{j}(-1)^j = \sum_{j=0}^{\infty}\binom{-1/2}{j},$$

which converges by the Leibniz criterion, the limit being given by Abel's limit theorem as $\lim_{s\uparrow 1}\sum_{j=0}^{\infty}\binom{-1/2}{j}s^j = \lim_{s\uparrow 1}(1+s)^{-1/2} = 2^{-1/2}$. Finally, by interchanging the summations in l and k and remembering that $F_\kappa(z) = 1 - G(z)$, we have proven our closed formula.

As in the case of negative z, a second formula for $F_\kappa(z)$ (with certain numerical advantages discussed in Section 4.4) can be obtained by choosing slightly different expansions in $l = 0, ..., j$ and $k = 0, ..., \infty$. The derivation of this second formula is analogous to that of the first formula, but with the sums in l and k modified in the same way as done when $z < 0$.

Theorem 2.15 *Let $z > 1/2$ and put $y := \sqrt{2z}$. The limiting distribution function of κ satisfies $F_\kappa(z) = -1 + \sum_{j=0}^{\infty} F_j(z)$ where the summand $F_j(z)$ has the two expressions:*

$$\begin{aligned} F_j(z) &= \sqrt{8y}\binom{j-1/2}{j}e^{y^2(j^2-j/2-7/16)}\sum_{k=0}^{\infty}y^k\sum_{l=0}^{j}\binom{j}{l}(-2y)^l \\ &\qquad\qquad\times\frac{D_{l+k+1/2}\left(y(2j+3/2)\right)}{\Gamma(l+k+3/2)} \\ &= \sqrt{8y}\binom{-1/2}{j}e^{y^2(j^2-j/2-7/16)}\sum_{k=0}^{\infty}c(j,k)y^k\frac{D_{k+1/2}((2j+3/2)y)}{\Gamma(k+3/2)}. \end{aligned}$$

Here $c(j,k)$ is given by (2.29) or Proposition 2.12 and equals 1 if $k \geq j$.

See Appendix A for the parabolic cylinder function $D_p(\zeta)$. As mentioned earlier, based on numerical tests the author believes that these formulae also hold when $0 < z \le 1/2$. By noting that $j^2 - j/2 - 7/16 = (2j+3/2)^2/4 - 2j - 1$, one can identify Abadir's hypergeometric function $K(p,\zeta) := e^{\zeta^2/4} D_p(\zeta)$ in both formulae.

2.3.5 Case of $z < 0$: a formula for $F_\kappa(z)$ involving a single series

Assume that $z < 0$. The formula to be derived here contains only one infinite series; this facilitates the numerical treatment.

In order to avoid the second infinite series (in k) we start with a different expansion of the integrand. First substituting $w = \sqrt{v}$ in (2.20),

$$F_\kappa(z) = \frac{1}{2\pi i} \int_{\sqrt{P_\varepsilon}} \frac{2}{w} e^{-w^2/z} \left[\cosh(2w) - \frac{w}{z}\sinh(2w)\right]^{-1/2} dw.$$

By Cauchy's theorem, the path $\sqrt{P_\varepsilon}$ can be replaced by the path $(b - i\infty, b + i\infty)$, where b is is arbitrary positive. The reason is that the integrand is holomorphic on $\operatorname{Re} w > 0$ and is of sufficiently small order as $|w| \to \infty$ and $|\arg w| \in [\pi/4, \pi/2]$. Now, we write $[\cosh(2w) - wz^{-1}\sinh(2w)]^{-1/2}$ as

$$\sqrt{2}\left(\frac{-z}{w}\right)^{1/2} e^{-w} \left(\frac{-z}{w} + \frac{-z}{w} e^{-4w} + 1 - e^{-4w}\right)^{-1/2},$$

which after choosing b sufficiently large that

$$\rho := \sup\left\{\left|\frac{-z}{w} + \frac{-z}{w}e^{-4w} - e^{-4w}\right| : w \in \mathbf{C} \text{ and } \operatorname{Re} w = b\right\} < 1, \tag{2.39}$$

can along $\operatorname{Re} w = b$ be expanded into the binomial series

$$\sqrt{2}\left(\frac{-z}{w}\right)^{1/2} e^{-w} \sum_{j=0}^{\infty} \binom{j-1/2}{j} (-)^j \left[\frac{-z}{w} + \frac{-z}{w}e^{-4w} - e^{-4w}\right]^j.$$

Hence $F_\kappa(z)$ has been brought into the form

$$F_\kappa(z) = \frac{1}{2\pi i} \int_{b-i\infty}^{b+i\infty} \sum_{j=0}^{\infty} g_j(z,w) dw \tag{2.40}$$

with

$$g_j(z,w) := 2\sqrt{2}\binom{j-1/2}{j}(-)^j \frac{1}{w} e^{-w^2/z}\left(\frac{-z}{w}\right)^{1/2}$$
$$\times\, e^{-w}\left[\frac{-z}{w} + \frac{-z}{w}e^{-4w} - e^{-4w}\right]^j. \tag{2.41}$$

Lemma 2.16 *In (2.40), summation and integration can be interchanged:*

$$F_\kappa(z) = \sum_{j=0}^{\infty} F_j(z) \quad \textit{with} \quad F_j(z) := \frac{1}{2\pi i}\int_{b-i\infty}^{b+i\infty} g_j(z,w)dw.$$

PROOF. In order to apply the dominated convergence theorem, note that, using (2.39),

$$|g_j(z,w)| < 2\sqrt{2}e^{-b^2/z}\sqrt{-z}|w|^{-3/2}\rho^j \quad \text{for } \operatorname{Re} w = b.$$

The claim follows from

$$\frac{1}{2\pi i}\int_{b-i\infty}^{b+i\infty}\sum_{j=0}^{\infty}|g_j(z,w)|dw < 2\sqrt{2}e^{-b^2/z}\sqrt{-z}\frac{1}{1-\rho}\frac{1}{2\pi i}\int_{b-i\infty}^{b+i\infty}|w|^{-3/2}dw$$
$$< \infty. \quad \textbf{QED}.$$

Theorem 2.17 *Let $z < 0$ and put $y := \sqrt{|2z|}$. The limiting distribution function is given by $F_\kappa(z) = \sum_{j=0}^{\infty} F_j(z)$ where*

$$F_j(z) := 2\sqrt{\frac{y}{\pi}}\binom{j-1/2}{j}\sum_{k=0}^{j}\binom{j}{k}(-y)^k\sum_{l=0}^{k}\binom{k}{l}$$
$$\times \exp(-(j+l-k+1/4)^2y^2)D_{-k-3/2}(2(j+l-k+1/4)y).$$

See Appendix A for the parabolic cylinder function $D_p(\zeta)$.

PROOF. To calculate the termwise integral $F_j(z)$ of Lemma 2.16 we expand (2.41), whereby $g_j(z,w)$ becomes

$$2\sqrt{2}\binom{j-1/2}{j}\frac{1}{w}e^{-w^2/z}\sum_{k=0}^{j}\binom{j}{k}(-)^k\left(\frac{-z}{w}\right)^{k+1/2}\sum_{l=0}^{k}\binom{k}{l}e^{-4(j+l-k+1/4)w}.$$

So we essentially have to calculate

$$\frac{1}{2\pi i}\int_{b-i\infty}^{b+i\infty} w^{-k-3/2}e^{-w^2/z}e^{-4(j+l-k+1/4)w}dw.$$

This integral is calculated in Lemma B.1, yielding the claimed formula. **QED**.

2.4 The t statistic

This section discusses closed expressions for the limiting distribution function $F_\tau(z)$ of the t ratio in our model. Section 2.4.1 treats the trivial (known) case $z = 0$. All following sections apply to the case $z < 0$, while the author (like Abadir) is unable to derive closed formulae when $z > 0$. Note that the case $z < 0$ is the more important one since it is needed to derive quantiles for testing against the alternatives $|\alpha| < 1$ (stationarity) or $\alpha < 1$, while the case $z > 0$ would be useful for the (less common) alternative of an explosive root $\alpha > 1$.

For $z < 0$ we discuss Abadir's (1995) and a new (cf. Dietrich, 2001) closed formula for $F_\tau(z)$, both contained in Theorem 2.22 (cf. Section 2.4.4). In the new formula the inner series has the numerically desirable Leibniz property. Regarding Abadir's derivation we prove a non-trivial interchangeability of integration and summation (cf. Section 2.4.2 and Appendix D), and present an alternative proof which avoids a step that is unclear to me (cf. Section 2.4.3). Finally, Section 2.4.5 gives an asymptotic expansion of $F_\tau(z)$ when $z \to -\infty$ (cf. Dietrich, 2001).

2.4.1 Case of $z = 0$

Like for $F_\kappa(0)$ (cf. Section 2.3.1), we have $F_\tau(0) = P(R/\sqrt{S} \leq 0) = P(R \leq 0)$, which by $R \overset{\mathcal{D}}{=} \chi^2(1)/2 - 1/2$ is the probability that a $\chi^2(1)$ variable is ≤ 1. So, as with $F_\kappa(0)$,

$$F_\tau(0) = \operatorname{erf}(2^{-1/2}) \approx 0.682689492137.$$

2.4.2 Case of $z < 0$: the limiting density $f_\tau(z)$ as a sum of integrals

From now on assume that $z < 0$. In Section 2.2 we have shown that (R, S) is absolutely continuous, and that (at least) for $(r, s) \in D := (-1/2, \infty) \times \mathbf{R}_+$ a (continuous) density is given by (2.18), viz.

$$f_{R,S}(r,s) := \frac{d}{dsdr}F_{R,S}(r,s) = \frac{1}{2\pi i}\int_{1+i\mathbf{R}} vg(v,r,s)dv, \quad (r,s) \in D \tag{2.42}$$

where $g(v,r,s)$ is given by (2.16). In this, the integrand $vg(v,r,s)$ possesses a Laplace transform with respect to $r > -1/2$, viz.

$$\int_{-1/2}^{\infty} e^{-ur}vg(v,r,s)dr = e^{sv+u/2}\left(\cosh\sqrt{2v} + \frac{u}{\sqrt{2v}}\sinh\sqrt{2v}\right)^{-1/2}.$$

In (2.42) write $vg(v,r,s)$ as the inverse of its Laplace transform:

$$f_{R,S}(r,s) = \frac{1}{2\pi i}\int_{1+i\mathbf{R}} e^{sv}\left\{\lim_{K\to\infty} \frac{1}{2\pi i}\int_{g_v-iK}^{g_v+iK} e^{(r+1/2)u}\left(\cosh\sqrt{2v} + \frac{u}{\sqrt{2v}}\sinh\sqrt{2v}\right)^{-1/2} du\right\} dv, \tag{2.43}$$

where the inversion integral is principal value integral which may be applied because the function $r \to vg(v,r,s)$ is continuous in $r > -1/2$ and of bounded variation in a neighbourhood of each $r > -1/2$. Note that the abscissa of integration, $g_v > 0$, may be chosen to depend on v. This formula, which – not surprisingly – consists in two Laplace inversion integrals applied to White's (1958) Laplace transform $E\{\exp(-uR - vS)\}$, forms the starting point of Abadir's (1995) derivation. After having proven the existence of a density $f_{R,S}(r,s)$ (Theorem 2.9), our detour through the expression (2.42) has been necessary to justify the use of the inversion formula (2.43).

From here, Abadir proceeds as follows. The transformation theorem for density functions yields the joint density of $(\tau, S) = (R/\sqrt{S}, S)$ as $f_{\tau,S}(z,s) = \sqrt{s}f_{R,S}(z\sqrt{s}, s)$. By integrating out the second variable, Abadir obtains the marginal density $f_\tau(z)$ as a triple integral: the outer integral coming from the marginalization and the two inner integrals being those in (2.43). As is discussed in Appendix D, in order to calculate these integrals Abadir first expands the integrand into a series and then applies all integrals summandwise; his expansion of the integrand is very similar to the starting expansion (2.23) in the derivations for κ. Up to a substitution, Abadir reaches the following expression:

Lemma 2.18 *(Abadir, 1995, p. 779) For all* $z < 0$,

$$f_\tau(z) = \frac{-2^{1/4}}{z^3} \sum_{j=0}^{\infty} \binom{j-1/2}{j} \sum_{l=0}^{j} \binom{j}{l} (-)^l 2^{l/2}$$
$$\frac{1}{2\pi i} \int_{b-i\infty}^{b+i\infty} \exp\left[\frac{v^2}{4z^2}\right] \exp\left[\frac{v}{\sqrt{2}}\right] v^{l+\frac{3}{2}} \Gamma\left(\frac{1}{2} - l, v\frac{4j+2}{\sqrt{2}}\right) dv.$$

Here, the integral resulting from the marginalization has been transformed into the incomplete gamma function, the integral with respect to v remains unsolved and the principal-value integral has been solved analytically. All of the interchanges of integrals with the summation or of two integrals can be shown to be correct. However, the interchangeability of the principle-value integral with the series is non-trivial; the principal-value integral in (2.43) is indeed an integral only in the principle-value sense since the integrand is *not* Lebesgue-integrable over $g_v + i\mathbf{R}$, and hence the dominated convergence theorem cannot apply. In Appendix D we give a (rather laborious) proof of this interchangeability.

2.4.3 Case of $z < 0$: the limiting distribution function $F_\tau(z)$ as a sum of integrals

Abadir transforms the density expression of Lemma 2.18 to finally obtain the formula contained in the following Theorem:

Theorem 2.19 *(Abadir, 1995, p. 781) If* $z < 0$ *then* $F_\tau(z) = \sum_{j=0}^{\infty} F_j(z)$ *where*

$$F_j(z) := \frac{2|z|}{\sqrt{\pi}} \binom{j-1/2}{j} \sum_{l=0}^{j} \binom{j}{l} (-2)^l \int_{4j+1}^{\infty} (s+1)^{-l-1/2} \exp\left[-\frac{1}{2}z^2 s^2\right] ds.$$

In this section we give a proof of Theorem 2.19 that differs from Abadir's derivation. Abadir begins by expanding $\Gamma(1/2 - l, v(4j+2)/\sqrt{2})$ in Lemma 2.18 into a diverging asymptotic expansion (as $v \to \infty$), and after applying some quite tricky, but intuitive transformations to the different summations he comes back to converging expressions. Unfortunately, I am unable to justify the validity of this procedure, however our proof given below avoids any unclarity.

By Lemma 2.18;

$$f_\tau(z) = 2^{1/4} \sum_{j=0}^{\infty} \binom{j-1/2}{j} \sum_{l=0}^{j} \binom{j}{l} \frac{(-)^l 2^{l/2}}{2\pi i} \int_{b-i\infty}^{b+i\infty} K_{jl}(z,v)\, dv \tag{2.44}$$

with

$$K_{jl}(z,v) := \frac{-1}{z^3} \exp\left[\frac{v^2}{4z^2}\right] \exp\left[\frac{v}{\sqrt{2}}\right] v^{l+\frac{3}{2}} \Gamma\left(\frac{1}{2} - l, v\frac{4j+2}{\sqrt{2}}\right).$$

The key to deriving the formula of Theorem 2.19 for $F_\tau(z) = \int_{-\infty}^{z} f_\tau(y)dy$ consists in recognizing $K_{jl}(z,v)$ as the product of two Laplace transforms, so that $K_{jl}(z,v)$ can be inverted via the convolution theorem:

Lemma 2.20 *For all $z < 0$ we have*

$$\frac{1}{2\pi i} \int_{b-i\infty}^{b+i\infty} K_{jl}(z,v)\, dv = \frac{2^{l/2-1/4}}{\sqrt{\pi}} \int_{4j+1}^{\infty} e^{-z^2 s^2/2} H_2\left(\frac{zs}{\sqrt{2}}\right) (s+1)^{-l-1/2} ds.$$

Proof. By a change of variable in the incomplete gamma function,

$$K_{jl}(z,v) = \frac{-1}{z^3} \exp\left[\frac{v^2}{4z^2}\right] \exp\left[\frac{v}{\sqrt{2}}\right] v^2 \int_{\frac{4j+2}{\sqrt{2}}}^{\infty} e^{-vt} t^{-l-1/2} dt.$$

Here, the function in front of the integral, say $g(v)$, is a Laplace transform[10] with inverse given by $\phi(t) := (2\pi i)^{-1} \int_{-i\infty}^{i\infty} e^{tv} g(v) dv$. By Lemma B.1, the inverse equals

$$\phi(t) = \frac{1}{\sqrt{\pi}} \exp\left[-z^2 \left(t + \frac{1}{\sqrt{2}}\right)^2\right] H_2\left[-z\left(t + \frac{1}{\sqrt{2}}\right)\right].$$

Hence $K_{jl}(z,v)$ is the product of a bilateral and a unilateral Laplace transform:

$$\int_{-\infty}^{\infty} \phi(t) e^{-vt} dt \cdot \int_{\frac{4j+2}{\sqrt{2}}}^{\infty} \psi(t) e^{-tv} dt, \quad \text{where} \quad \psi(t) := t^{-l-1/2}.$$

[10] This follows from the fact that $g(iv)$ is a Schwartz function, where we use that Fourier transformation defines a bijection between the Schwartz space onto itself with inverse given by the Fourier inversion integral.

The convolution theorem now implies that $K_{jl}(z,v)$ is the Laplace transform of the convolution

$$(\phi * \psi)(t) = \int_{\frac{4j+2}{\sqrt{2}}}^{\infty} \phi(t-s)\psi(s)ds.$$

Since $\phi * \psi$ is continuous and of bounded variation[11] (at least) in a neighbourhood of $t=0$, its value in $t=0$ can be obtained via the Laplace inversion integral:

$$\frac{1}{2\pi i}\int_{b-i\infty}^{b+i\infty} K_{jl}(z,v)\,dv = (\phi * \psi)(0) = \int_{\frac{4j+2}{\sqrt{2}}}^{\infty} \phi(-s)\psi(s)ds,$$

which by substitution $2^-1/2(s+1)$ for s yields the desired expression. **QED.**

Now the density (2.44) becomes

$$f_\tau(z) = \frac{1}{\sqrt{\pi}}\sum_{j=0}^{\infty}\binom{j-1/2}{j}\sum_{l=0}^{j}\binom{j}{l}(-2)^l S_{jl}(z) \tag{2.45}$$

where

$$S_{jl}(z) := \int_{4j+1}^{\infty} \exp\left[-\frac{1}{2}z^2s^2\right] H_2\left(\frac{zs}{\sqrt{2}}\right)(s+1)^{-l-1/2}ds.$$

We wish to calculate the distribution function $F_\tau(z) = \int_{-\infty}^{z} f_\tau(z')dz'$. In Appendix E we prove that the integral in z' can be interchanged first with the infinite sum (Lemma E.1) and then with the integral occurring in $S_{jl}(z)$ (Lemma E.2). Then

$$F_\tau(z) = \frac{1}{\sqrt{\pi}}\sum_{j=0}^{\infty}\binom{j-1/2}{j}\sum_{l=0}^{j}\binom{j}{l}(-2)^l \int_{4j+1}^{\infty} ds(s+1)^{-l-1/2}$$
$$\times \int_{-\infty}^{z} \exp\left[-\frac{1}{2}z'^2s^2\right] H_2\left(\frac{z's}{\sqrt{2}}\right)dz',$$

where the last integral in z' by a simple substitution becomes

$$\frac{\sqrt{2}}{s}\int_{-\infty}^{\frac{zs}{\sqrt{2}}} \exp\left[-z'^2\right] H_2(z')dz' = \frac{\sqrt{2}}{s}\int_{-\infty}^{\frac{zs}{\sqrt{2}}} \frac{d^2}{dz'^2}\exp\left[-z'^2\right]dz'$$
$$= -2z\exp\left[-\frac{1}{2}z^2s^2\right].$$

This proves the formula of Theorem 2.19.

[11] This can be seen by showing that $\frac{d}{dt}(\phi * \psi)(t)$ is bounded in a neighbourhood of $t=0$.

2.4.4 Case of $z < 0$: Abadir's and a new closed formula for $F_\tau(z)$

We now complete the derivation of Abadir's formula (1995) and of the new closed formula with the desirable Leibniz series (Dietrich, 2001, Section 2). These two formulae are contained in Theorem 2.22 below.

While the derivation of both formulae have been identical up to the expression of Theorem 2.19, they differ from now on. To obtain his expression, Abadir writes the remaining integral in Theorem 2.19 as

$$\int_{4j+2}^{\infty} s^{-l-1/2} e^{-z^2(1-2s+s^2)/2} ds = e^{-z^2/2} \int_{4j+2}^{\infty} \sum_{k=0}^{\infty} \frac{z^{2k}}{k!} s^{k-l-1/2} e^{-z^2 s^2/2} ds$$

which by the monotone convergence theorem becomes

$$e^{-x^2/4} 2^{-l-1/2} x^{l-1/2} \sum_{k=0}^{\infty} \frac{x^k}{k!} \Gamma\left(\frac{1}{4} + \frac{k}{2} - \frac{l}{2}, x^2(2j+1)^2\right), \tag{2.46}$$

where $x := 2^{1/2}|z|$.

To derive the new closed formula for $F_j(z)$, we apply the binomial formula to the sum in Theorem 2.19, thereby obtaining

$$F_j(z) = \frac{2|z|}{\sqrt{\pi}} \binom{j-1/2}{j} L_j(z) \tag{2.47}$$

with

$$L_j(z) := \int_{4j+1}^{\infty} \frac{[1 - 2(s+1)^{-1}]^j}{(s+1)^{1/2}} \exp\left[-\frac{1}{2} z^2 s^2\right] ds. \tag{2.48}$$

Now we transform the fraction in $L_j(z)$ via another binomial expansion into

$$\frac{(s-1)^j}{(s+1)^{j+1/2}} = s^{-1/2} \frac{(1-s^{-1})^j}{(1+s^{-1})^{j+1/2}} = \sum_{k=0}^{\infty} \binom{-j-1/2}{k} s^{-1/2-k} (1-s^{-1})^j.$$

So

$$L_j(z) = \int_{4j+1}^{\infty} \sum_{k=0}^{\infty} u_k(s) ds$$

with

$$u_k(s) := u_k(s, j, z) := \binom{-j-1/2}{k} s^{-1/2-k} (1-s^{-1})^j \exp\left[-\frac{1}{2} z^2 s^2\right].$$

The next lemma will, amongst other things, allow us to integrate termwise in $L_j(z)$.

Lemma 2.21 *Let $s > 4j+1$. Then $\sum_{k=0}^{\infty} u_k(s)$ is a Leibniz series; more precisely, $((-)^k u_k(s))_{k\in\mathbf{N}}$ is positive and strictly decreasing to 0. In particular the series is dominated by $u_0(s)$, so that by the dominated convergence theorem and with $y := 2^{-1/2}|z|$*

$$L_j(z) = \sum_{k=0}^{\infty} \int_{4j+1}^{\infty} u_k(s)ds = \frac{1}{2}\sum_{k=0}^{\infty} \binom{-j-1/2}{k} y^{k-1/2} \sum_{l=0}^{j} \binom{j}{l} (-y)^l$$

$$\Gamma\left(\frac{1}{4} - \frac{l}{2} - \frac{k}{2}, y^2(4j+1)^2\right). \tag{2.49}$$

PROOF. We have

$$(-)^k u_k(s) = \left|\binom{-j-1/2}{k}\right| s^{-1/2-k}(1-s^{-1})^j \exp[-y^2 s^2],$$

so that $(-)^k u_k(s)$ is positive. Also, by $s > 4j+1$

$$\begin{aligned}
(-)^{k+1} u_{k+1}(s) &< \left|\binom{-j-1/2}{k+1}\right| \frac{s^{-1/2-k}}{4j+1}(1-s^{-1})^j \exp[-y^2 s^2] \\
&= \frac{j+1/2+k}{k+1} \left|\binom{-j-1/2}{k}\right| \frac{s^{-1/2-k}}{4j+1}(1-s^{-1})^j \exp[-y^2 s^2] \\
&= \frac{j+1/2+k}{(k+1)4j+k+1}(-)^k u_k(s) \\
&< (-)^k u_k(s).
\end{aligned}$$

So $((-)^k u_k(s))_{k\in\mathbf{N}}$ is strictly decreasing, the limit being 0 because otherwise $\sum_{k=0}^{\infty} u_k(s)$ would diverge.

The dominating function $u_0(s)$ obviously has a finite integral over $[4j+1, \infty[$, so that termwise integration is permissible. Formula (2.49) follows by expressing $\int_{4j+1}^{\infty} u_k(s)ds$ in terms of the incomplete gamma function, which is achieved by writing $(1-s^{-1})^j = \sum_{l=0}^{j} \binom{j}{l}(-)^l s^{-l}$ and substituting $t = y^2 s^2$. **QED.**

The result of this section can now be proven.

Theorem 2.22 *Let $z < 0$. The limiting distribution function of τ is given by $F_\tau(z) = \sum_{j=0}^{\infty} F_j(z)$, where the summand $F_j(z)$ has the two following expressions:*

$$F_j(z) = \sqrt{\frac{x}{\pi}} e^{-x^2/4} \binom{j-1/2}{j} \sum_{k=0}^{\infty} \frac{x^k}{k!} \sum_{l=0}^{j} \binom{j}{l} (-x)^l$$

$$\times \Gamma\left(\frac{1}{4} - \frac{l}{2} + \frac{k}{2}, x^2(2j+1)^2\right), \quad x := 2^{1/2}|z|, \tag{2.50}$$

$$= \sqrt{\frac{2y}{\pi}} \binom{j-1/2}{j} \sum_{k=0}^{\infty} \binom{-j-1/2}{k} y^k \sum_{l=0}^{j} \binom{j}{l} (-y)^l$$

$$\times \Gamma\left(\frac{1}{4} - \frac{l}{2} - \frac{k}{2}, y^2(4j+1)^2\right), \quad y := 2^{-1/2}|z|. \tag{2.51}$$

In (2.51), the series in k is a Leibniz series; more precisely, putting

$$\gamma_{jk}(z) := \binom{-j-1/2}{k} y^k \sum_{l=0}^{j} \binom{j}{l} (-y)^l \Gamma\left(\frac{1}{4} - \frac{l}{2} - \frac{k}{2}, y^2(4j+1)^2\right),$$

the sequence $((-)^k \gamma_{jk}(z))_{k\in\mathbf{N}}$ is positive and strictly decreasing to 0, so that the truncation error is bounded by $|\sum_{k=K}^{\infty} \gamma_{jk}(z)| < |\gamma_{jK}(z)|$ for all $K \in \mathbf{N}$.

PROOF. The formulae for $F_j(z)$ follow from the above derivations: In the non-closed expression of Theorem 2.19, replace the integral by (2.46) to obtain Abadir's formula (2.50), or replace the sum $L_j(z)$ by its expression of Lemma 2.21 to obtain the new formula (2.51).

Regarding the Leibniz property, we can equivalently show that

$$\sum_{k=0}^{\infty} 2^{-1} y^{-1/2} \gamma_{jk}(z)$$

is a Leibniz series. This series is nothing other than the series

$$\sum_{k=0}^{\infty} \int_{4j+1}^{\infty} u_k(s) ds$$

of Lemma 2.21 (where $u_k(s)$ depends on j, z). By this lemma, $((-)^k u_k(s))_{k\in\mathbf{N}}$ is positive and strictly decreasing to 0. So the same is true for the integrated sequence $\left((-)^k \int_{4j+1}^{\infty} u_k(s) ds\right)_{k\in\mathbf{N}}$. **QED.**

2.4.5 An asymptotic expansion of $F_\tau(z)$ as $z \to -\infty$

Using an expansion of Abadir (1995), this section (cf. Dietrich, 2001, Section 5) derives an asymptotic expansion of the form

$$F_\tau(z) \sim e^{-z^2/4} \sum_{k=0}^{\infty} a_k z^{-k} D_{-k-1}(|z|) \quad \text{as } z \to -\infty$$

for certain coefficients $a_k \in \mathbf{R}$.

By expanding asymptotically the incomplete gamma function in Lemma 2.18, Abadir (1995, p. 780, (2.10)) derives an asymptotic expansion of $F_j(z)$ as $z \to -\infty$. For $j = 0$ this expansion is given by

$$F_0(z) = \sqrt{\frac{2}{\pi}} e^{-z^2/4} \left\{ \sum_{k=0}^{K-1} \frac{(1/2)_k}{(2z)^k} D_{-k-1}(|z|) + O\left(|z|^{-K} D_{-K-1}(|z|)\right) \right\} \tag{2.52}$$

as $z \to -\infty$, where $K \in \mathbf{N}$. We will see that $F_\tau(z)$ has exactly the same expansion as $F_0(z)$.

First we add $\sum_{j=1}^{\infty} F_j(z)$ to both sides of (2.52), which yields

$$\begin{aligned} F_\tau(z) = {} & \sum_{j=1}^{\infty} F_j(z) \\ & + \sqrt{\frac{2}{\pi}} e^{-z^2/4} \left\{ \sum_{k=0}^{K-1} \frac{(1/2)_k}{(2z)^k} D_{-k-1}(|z|) + O\left(|z|^{-K} D_{-K-1}(|z|)\right) \right\}. \end{aligned} \tag{2.53}$$

On the right hand side the term $\sum_{j=1}^{\infty} F_f(z)$ is asymptotically of smaller order than the residual:

$$\sum_{j=1}^{\infty} F_j(z) = o\left(e^{-z^2/4} |z|^{-K} D_{-K-1}(|z|)\right) \quad \text{as } z \to -\infty. \tag{2.54}$$

This is because a bound derived later for $\sum_{j=J}^{\infty} F_j(z)$ (Proposition 3.1) implies that $\sum_{j=1}^{\infty} F_j(z) = o(\exp(-25z^2/2))$, and because

$$D_\nu(a) \sim e^{-a^2/4} a^\nu \quad \text{as } a \to \infty \tag{2.55}$$

(Gradshteyn and Ryzhik, 1994, p. 1093, 9.246 (1)). By (2.54) the term $\sum_{j=1}^{\infty} F_j(z)$ can be dropped in (2.53):

Proposition 2.23 *$F_\tau(z)$ has for all $K \in \mathbf{N}$ the asymptotic representation*

$$F_\tau(z) = \sqrt{\frac{2}{\pi}} e^{-z^2/4} \left\{ \sum_{k=0}^{K-1} \frac{(1/2)_k}{(2z)^k} D_{-k-1}(|z|) + R_K(z) \right\}$$

where the residual satisfies

$$R_K(z) = O\left(|z|^{-K} D_{-K-1}(|z|)\right) = O\left(|z|^{-2K-1} e^{-z^2/4}\right) \quad \text{as } z \to -\infty.$$

PROOF. The first expression for the order of $R_K(z)$ has been proven and the second expression follows from (2.55). **QED.**

Taking $K = 1$ we obtain that, as noted by Abadir (1995, p. 782), the lower tail of the distribution has twice the thickness of the lower tail of the standard normal distribution:

Corollary 2.24 *If $\Phi(z)$ denotes the standard normal distribution function,*

$$F_\tau(z) \sim \sqrt{\frac{2}{\pi}} e^{-z^2/4} D_{-1}(|z|) = 2\Phi(z) \sim \sqrt{\frac{2}{\pi}} e^{-z^2/2} |z|^{-1} \quad \text{as } z \to -\infty.$$

PROOF. The two equivalences follow from the Proposition 2.23 and (2.55). The equality follows from Gradshteyn and Ryzhik (1994, p. 1095, 9.254 (1)). **QED.**

2.5 The limiting densities of τ and κ

The derived expressions for $F_\tau(z)$ and $F_\kappa(z)$ can be differentiated to yield expressions for the densities $f_\tau(z)$ and $f_\kappa(z)$. These density expressions contain the same number of infinite summations as the corresponding distribution function expressions, but lose in simplicity and elegance.

After proving the differentiability of $F_\tau(z)$ and $F_\kappa(z)$ and the interchangeability of differentiation and summation(s), the technical differentiation is a straightforward exercise. In the differentiation of $F_\tau(z)$ one should use that $\frac{d}{d\zeta}\Gamma(p,\zeta) = -\zeta^{p-1}e^{-\zeta}$. In that of $F_\kappa(z)$ one should identify (in each expression) Abadir's function $K_p(\zeta) = e^{-\zeta^2/4} D_p(\zeta)$ which has a simple derivative, namely

$$\frac{d}{d\zeta} K(p,\zeta) = e^{\zeta^2/4} \left\{ \zeta D_p(\zeta)/2 + \frac{d}{d\zeta} D_p(\zeta) \right\} = pK(p-1,\zeta)$$

by a functional relation for $D_p(\zeta)$ (Gradshteyn and Ryzhik, 1994, p. 1094).

As an example, we here calculate $f_\tau(z)$, the procedure for $f_\kappa(z)$ being analogous. The first expression for $f_\tau(z)$ in each Proposition 2.25 and Corollary 2.26 is found by Abadir (1995, p. 782, (2.12)) by differentiating his expression (2.50) for $F_\tau(z)$. The second expression (Dietrich, 2001, Section 6) is both times obtained from our new expression for $F_\tau(z)$.

Proposition 2.25 *$F_\tau(z)$ is continuously differentiable on $z \in \mathbf{R}_-$. The limiting density is given as $f_\tau(z) = \sum_{j=0}^\infty f_j(z)$ where $f_j(z)$ has the two expressions*

$$\begin{aligned} f_j(z) = {} & \sqrt{\frac{2}{\pi}} e^{-x^2/4} \binom{j-1/2}{j} \sum_{k=0}^{\infty} \frac{x^k}{k!} \sum_{l=0}^{j} \binom{j}{l} (-)^l \\ & \times \left\{ 2x^k (2j+1)^{k-l+1/2} e^{-x^2(2j+1)^2} + \left(\frac{x^2}{2} - l - k - \frac{1}{2} \right) x^{l-1/2} \right. \\ & \left. \times \Gamma\left(\frac{1}{4} - \frac{l}{2} + \frac{k}{2}, x^2(2j+1)^2 \right) \right\}, \quad x := 2^{1/2}|z|, \qquad (2.56) \\ = {} & \frac{1}{\sqrt{\pi}} \binom{j-1/2}{j} \sum_{k=0}^{\infty} \binom{-j-1/2}{k} \sum_{l=0}^{j} \binom{j}{l} (-)^l \\ & \times \left\{ 2(4j+1)^{1/2-l-k} e^{-y^2(4j+1)^2} - \left(k + l + \frac{1}{2} \right) y^{k+l-1/2} \right. \\ & \left. \times \Gamma\left(\frac{1}{4} - \frac{l}{2} - \frac{k}{2}, y^2(4j+1)^2 \right) \right\}, \quad y := 2^{-1/2}|z|. \qquad (2.57) \end{aligned}$$

PROOF. The two expressions (2.56) and (2.57) are obtained by writing the formula (2.50) respectively (2.51) for $F_j(z)$ as $\sum_{k=0}^\infty F_{jk}(z)$ (with $F_{jk}(z)$ depending on the formula), and then computing $\frac{d}{dz} F_\tau(z) = \sum_{j=0}^\infty \sum_{k=0}^\infty \frac{d}{dz} F_{jk}(z)$. This however supposes that $F_\tau(z)$ is differentiable and that differentiation is interchangeable with two summations. We prove these statements, using an argument of complex analysis. The argument is analogous for both formulae for $F_j(z)$, so we consider for instance Abadir's formula (2.50). Here

$$F_{jk}(z) = \sqrt{\frac{x}{\pi}} e^{-x^2/4} \binom{j-1/2}{j} \frac{x^k}{k!} \sum_{l=0}^{j} \binom{j}{l} (-x)^l \Gamma\left(\frac{1}{4} - \frac{l}{2} + \frac{k}{2}, x^2(2j+1)^2 \right)$$

with $x := 2^{1/2}|z|$. We use the argument that the locally uniform limit[12] of **C**-differentiable (i.e. holomorphic) functions on some region $D \subset \mathbf{C}$ is again **C**-differentiable, with derivative the limit of the derivatives (by Weierstrass' Theorem, cf. Ahlfors (1966), p. 174), while the parallel statement for **R**-differentiable functions would need additional conditions. The above equation defines an analytic continuation of $F_{jk}(z)$ on

$$z \in D := \{\zeta \in \mathbf{C} |\, \mathrm{Re}\, \zeta < 0 \text{ and } \mathrm{Re}\, \zeta^2 > 0\},$$

the original domain of $F_{jk}(z)$ being $]-\infty, 0[= D \cap \mathbf{R}$. Further, one can prove that the series $\sum_{k=0}^{\infty} F_{jk}(z)$ is locally uniformly convergent on D, so that the limit $F_j(z) = \sum_{k=0}^{\infty} F_{jk}(z)$ is also analytic on D and termwise **C**-differentiable:

$$\frac{d}{dz} F_j(z) = \sum_{j=0}^{\infty} \frac{d}{dz} \left\{ F_{jk}(z) \right\}, \quad z \in D. \tag{2.58}$$

The next step is analogous. One shows the locally uniform convergence of $\sum_{j=0}^{\infty} F_j(z)$ on D, which implies that the limit $F_\tau(z) = \sum_{j=0}^{\infty} F_j(z)$ is also analytic on D and termwise **C**-differentiable:

$$\frac{d}{dz} F_\tau(z) = \sum_{j=0}^{\infty} \frac{d}{dz} \left\{ F_j(z) \right\}, \quad z \in D. \tag{2.59}$$

Formulae (2.58) and (2.59) together imply $\frac{d}{dz} F_\tau(z) = \sum_{j=0}^{\infty} \sum_{k=0}^{\infty} \frac{d}{dz} F_{jk}(z)$, in the sense of **C**-differentiation on D. In particular the equation holds in the sense of **R**-differentiation on $]-\infty, 0[$. **QED.**

In each density expression (2.56) and (2.57) the inner series in k has very complicated summands. In both expressions, a simplification can be achieved by splitting the inner series as in the below corollary.

Corollary 2.26 *With the notation of Proposition 2.25, the density summand*

[12] A sequence of functions $G_n(z)$ converges "locally uniformly" on $z \in D$ to a function $G(z)$ if each $z_0 \in D$ posseses a neighbourhood $z_0 \in D_0 \subseteq D$ such that $\sup\{|G(z) - G_n(z)| : z \in D_0\} \to 0$.

$f_j(z)$ *has the expressions*

$$f_j(z) = \sqrt{\frac{2}{\pi}} e^{-x^2/4} \binom{j-1/2}{j} \left\{ \frac{2^{3/2} j^j}{(j+1/2)^{j-1/2}} e^{-2jx^2(2j+1)} + \frac{1}{\sqrt{x}} \sum_{k=0}^{\infty} \frac{x^k}{k!} \right.$$
$$\left. \times \sum_{l=0}^{j} \binom{j}{l} (-x)^l \left(\frac{x^2}{2} - l - k - \frac{1}{2} \right) \Gamma\left(\frac{1}{4} - \frac{l}{2} + \frac{k}{2}, x^2(2j+1)^2 \right) \right\}$$
$$= \frac{1}{\sqrt{\pi}} \binom{j-1/2}{j} \left\{ \frac{j^j(4j+1)}{(j+1/2)^{j+1/2}} e^{-y^2(4j+1)^2} - \sum_{k=0}^{\infty} \binom{-j-1/2}{k} \right.$$
$$\left. \times \sum_{l=0}^{j} \binom{j}{l} (-)^l \left(k + l + \frac{1}{2} \right) y^{k+l-1/2} \Gamma\left(\frac{1}{4} - \frac{l}{2} - \frac{k}{2}, y^2(4j+1)^2 \right) \right\}$$

where j^j *is defined as* 1 *if* $j = 0$.

PROOF. We derive the first expression from (2.56), the second follows similarly from (2.57). By a sum reordering[13], (2.56) becomes

$$f_j(z) = \sqrt{\frac{2}{\pi}} e^{-x^2/4} \binom{j-1/2}{j} \left\{ T_j(z) + \frac{1}{\sqrt{x}} \sum_{k=0}^{\infty} \frac{x^k}{k!} \sum_{l=0}^{j} \binom{j}{l} (-x)^l \right.$$
$$\left. \times \left(\frac{x^2}{2} - l - k - \frac{1}{2} \right) \Gamma\left(\frac{1}{4} - \frac{l}{2} + \frac{k}{2}, x^2(2j+1)^2 \right) \right\},$$

where $T_j(z)$ is

$$\sum_{k=0}^{\infty} \frac{x^k}{k!} \sum_{l=0}^{j} \binom{j}{l} (-)^l 2x^k (2j+1)^{k-l+1/2} e^{-x^2(2j+1)^2} = 2^{3/2} \frac{j^j e^{-2jx^2(2j+1)}}{(j+1/2)^{j-1/2}}. \textbf{ QED}.$$

[13] In general, $\sum_k (a_k + b_k) = \sum_k a_k + \sum_k b_k$ provided that two (and therefore all three) of the occuring series converge; here $\sum_k a_k$ is the series $T_j(z)$, which is indeed convergent.

Chapter 3

Bounds for Series Truncation Errors

This chapter derives upper bounds for the errors produced by truncating series occurring in the formulae derived in Chapter 2 for the distribution functions of the asymptotic test statistics τ (cf. Dietrich, 2001, Section 3) and κ (cf. Dietrich, 2002b). Unlike in Chapter 2, we here first consider τ (cf. Section 3.1) and then κ (cf. Section 3.2), since the discussion for τ seems easier.

The numerical implementation built on these error bounds is discussed in the following Chapter 4.

3.1 Truncation error bounds for the t statistic

We consider the expressions for $F_\tau(z)$ of Theorem 2.22. There, $F_\tau(z)$ is for $z < 0$ written as a series $\sum_{j=0}^{\infty} F_j(z)$, where for $F_j(z)$ two series expressions (in k) are given, the first of which is by Abadir (1993). Proposition 3.1 contains an error inequality for the series in j and for Abadir's series in k. Note that the other series in k is Leibniz and hence already possesses a comfortable truncation error bound (Theorem 2.22). As a by-product we derive an upper bound for $F_\tau(z)$ itself (Corollary 3.2). Finally, we derive a simplified, but weaker error bound for Abadir's series in k (Corollary 3.3).

Proposition 3.1 *Let $z < 0$ and consider the series $F_\tau(z) = \sum_{j=0}^{\infty} F_j(z)$ of Theorem 2.22. We have $F_j(z) > 0$, and for all $J \in \mathbf{N}$ the truncation error*

satisfies
(3.1)

$$0 < \sum_{j=J}^{\infty} F_j(z) < \frac{2(4J+1)^{-3/2}}{|z|\sqrt{\pi}} \binom{J-1/2}{J} e^{-z^2(4J+1)^2/2} \left(1 - e^{-4z^2(4J+1)}\right)^{-1}.$$

Now consider in Abadir's expression (2.50) *for* $F_j(z)$ *the inner series* $\sum_{k=0}^{\infty} \delta_{jk}(z)$ *where*

$$\delta_{jk}(z) := \frac{x^k}{k!} \sum_{l=0}^{j} \binom{j}{l} (-x)^l \Gamma\left(\frac{1}{4} - \frac{l}{2} + \frac{k}{2}, x^2(2j+1)^2\right), \quad x := 2^{1/2}|z|.$$

Then $\delta_{jk}(z) > 0$, *and provided that* $K = 1, 2, ...$ *an upper truncation error bound which is independent of* j *is given by*

$$0 < \sum_{k=K}^{\infty} \delta_{jk}(z) < 2^{3/4} e^{z^2/4} \frac{|z|^K}{\sqrt{K}} D_{-K-1/2}(z). \tag{3.2}$$

See Appendix A for the parabolic cylinder function $D_p(\zeta)$.

Proof: *Bound (3.1).* To dominate $F_j(z)$, we write $F_j(z)$ as in (2.47)-(2.48):

$$F_j(z) = \frac{2|z|}{\sqrt{\pi}} \binom{j-1/2}{j} L_j(z) \tag{3.3}$$

with

$$L_j(z) = \int_{4j+1}^{\infty} \frac{[1 - 2(s+1)^{-1}]^j}{(s+1)^{1/2}} \exp\left[-\frac{1}{2} z^2 s^2\right] ds.$$

So, by $2(s+1)^{-1} < 1$ we have $0 < L_j(z)$ and hence $0 < \sum_{j=J}^{\infty} F_j(z)$; moreover,

$$L_j(z) < \int_{4j+1}^{\infty} \frac{e^{-z^2 s^2/2}}{s^{1/2}} ds = \frac{2^{-3/4}}{\sqrt{|z|}} \int_{z^2(4j+1)^2/2}^{\infty} \frac{e^{-t}}{t^{3/4}} dt < \frac{e^{-z^2(4j+1)^2/2}}{z^2(4j+1)^{3/2}},$$

and hence

$$\begin{aligned} \sum_{j=J}^{\infty} F_j(z) &< \frac{2}{|z|\sqrt{\pi}} \sum_{j=J}^{\infty} \binom{j-1/2}{j} \frac{e^{-z^2(4j+1)^2/2}}{(4j+1)^{3/2}} \\ &< \frac{2(4J+1)^{-3/2}}{|z|\sqrt{\pi}} \binom{J-1/2}{J} \sum_{j=0}^{\infty} e^{-z^2(4j+4J+1)^2/2}, \end{aligned} \tag{3.4}$$

in which

$$\sum_{j=0}^{\infty} e^{-z^2(4j+4J+1)^2/2} = e^{-z^2(4J+1)^2/2} \sum_{j=0}^{\infty} e^{-z^2 8j(4J+1)/2}$$
$$= e^{-z^2(4J+1)^2/2} \left(1 - e^{-4z^2(4J+1)}\right)^{-1}.$$

Bound (3.2). Consider Abadir's inner series. We have

$$\begin{aligned} 0 < \delta_{jk}(z) &= \frac{x^k}{k!} \int_{x^2(2j+1)^2}^{\infty} \left(1 - xt^{-1/2}\right)^j t^{k/2-3/4} e^{-t} dt \\ &< \frac{x^k}{k!} \int_{x^2(2j+1)^2}^{\infty} t^{k/2-3/4} e^{-t} dt \\ &< \frac{x^k}{k!} \int_0^{\infty} t^{k/2-3/4} e^{-t} dt \end{aligned}$$

where the two first inequalities follow from $0 < xt^{-1/2} < 1$. So

$$\begin{aligned} 0 < \sum_{k=K}^{\infty} \delta_{jk}(z) &< \sum_{k=K}^{\infty} \frac{x^k}{k!} \int_0^{\infty} t^{k/2-3/4} e^{-t} dt \\ &< \frac{x^K}{K!} \sum_{k=0}^{\infty} \frac{x^k}{k!} \int_0^{\infty} t^{(K+k)/2-3/4} e^{-t} dt. \end{aligned}$$

Applying the monotone convergence theorem to the last expression, we deduce

$$\sum_{k=K}^{\infty} \delta_{jk}(z) < \frac{x^K}{K!} \int_0^{\infty} t^{K/2-3/4} \sum_{k=0}^{\infty} \frac{x^k t^{k/2}}{k!} e^{-t} dt = \frac{x^K}{K!} \int_0^{\infty} t^{K/2-3/4} e^{x\sqrt{t}-t} dt.$$

After a substitution, the last expression can be represented in terms of the parabolic cylinder function, so that we have

$$\begin{aligned} \sum_{k=K}^{\infty} \delta_{jk}(z) &< 2^{3/4} \frac{|z|^K}{K!} \int_0^{\infty} s^{K-1/2} e^{-zs-s^2/2} ds \\ &= 2^{3/4} e^{z^2/4} \frac{|z|^K \Gamma(K+1/2)}{K!} D_{-K-1/2}(z). \end{aligned}$$

(Gradshteyn and Ryzhik, 1994, p. 1092, 9.241 (2)). The bound (3.2) follows by dominating $\Gamma(K+1/2)$ according to the convexity of the log-gamma function:

$$\Gamma(K+1/2) < \sqrt{\Gamma(K)\Gamma(K+1)} = (K-1)!\sqrt{K}. \quad \textbf{QED}.$$

If in the truncation error bound (3.1) for $\sum_{j=J}^{\infty} F_j(z)$ we put $J = 0$, the truncation error becomes $\sum_{j=0}^{\infty} F_j(z)$, i.e. $F_\tau(z)$ itself, so that (3.1) is a bound for $F_\tau(z)$. This bound can be strengthened by slightly modifying the above proof in the case of $J = 0$:

Corollary 3.2 *For all $z < 0$,*

$$F_\tau(z) < \frac{2}{|z|\sqrt{\pi}} e^{-z^2/2} \left(1 - e^{-4z^2}\right)^{-1/2}.$$

Proof. If $J = 0$, then by (3.4) we have

$$\begin{aligned} F_\tau(z) = \sum_{j=0}^{\infty} F_j(z) &< \frac{2}{|z|\sqrt{\pi}} \sum_{j=0}^{\infty} \binom{-1/2}{j} (-)^j \frac{e^{-z^2(4j+1)^2/2}}{(4j+1)^{3/2}} \\ &< \frac{2}{|z|\sqrt{\pi}} e^{-z^2/2} \sum_{j=0}^{\infty} \binom{-1/2}{j} (-)^j e^{-z^2 4j} \\ &= \frac{2}{|z|\sqrt{\pi}} e^{-z^2/2} \left(1 - e^{-4z^2}\right)^{-1/2}. \quad \textbf{QED}. \end{aligned}$$

We now see that our bound (3.2) for $\sum_{k=K}^{\infty} \delta_{jk}(z)$ can be weakened so as to avoid the higher transcendental function $D_{-K-1/2}(z)$. If $|z|$ is relatively small, the loss of strength of the simplified bound is small or moderate. But if $|z|$ becomes large then the new bound is less useful since K has to become extremely large before the bound starts converging to 0.

Note first that

$$\begin{aligned} D_{-K-1/2}(z) = \frac{\sqrt{\pi}\exp(-z^2/4)}{2^{K/2+1/4}} \Bigg[&\frac{1}{\Gamma(K/2+3/4)} {}_1F_1\left(\frac{K}{2}+\frac{1}{4}, \frac{1}{2}; \frac{z^2}{2}\right) \\ &+ \frac{\sqrt{2}|z|}{\Gamma(K/2+1/4)} {}_1F_1\left(\frac{K}{2}+\frac{3}{4}, \frac{3}{2}, \frac{z^2}{2}\right) \Bigg] \end{aligned}$$

(cf. Appendix A). So, since

$${}_1F_1(a,b,y) = \sum_{n=0}^{\infty} \frac{(a)_n}{(b)_n n!} y^n \le \sum_{n=0}^{\infty} \frac{a^n}{b^n n!} y^n = \exp\left[\frac{a}{b} y\right] \text{ if } a \ge b > 0 \text{ and } y > 0,$$

we have for all $K \geq 2$

$$D_{-K-1/2}(z) \leq \frac{\sqrt{\pi}\exp(-z^2/4)}{2^{K/2+1/4}} \times \left[\frac{\exp\left[(K/2+1/4)z^2\right]}{\Gamma(K/2+3/4)} + \frac{\sqrt{2}|z|\exp\left[(K/6+1/4)z^2\right]}{\Gamma(K/2+1/4)}\right].$$

Using this inequality, the bound (3.2) can be weakened as follows:

Corollary 3.3 *If $K = 2, 3, \ldots$ an upper bound that is independent of j is*

$$0 < \sum_{k=K}^{\infty} \delta_{jk}(z) < \frac{\sqrt{\pi}|z|^K}{2^{K/2-1/2}\sqrt{K}} \times \left[\frac{\exp\left[(K/2+1/4)z^2\right]}{\Gamma(K/2+3/4)} + \frac{\sqrt{2}|z|\exp\left[(K/6+1/4)z^2\right]}{\Gamma(K/2+1/4)}\right].$$

3.2 Truncation error bounds for the normalised coefficient estimator

This section discusses truncation error bounds for the various series expressions derived for $F_\kappa(z)$ (cf. Section 2.3). Section 3.2.1 derives bounds for the expressions for $z < 0$ involving two infinite series. Section 3.2.2 briefly discusses the expressions for $z > 0$, where the author is unable to find a truncation error bound for the outer series. Finally, Section 3.2.3 treats the expression for $z < 0$ involving only one infinite series.

3.2.1 Case of $z < 0$: series truncation in Theorem 2.11

We consider the truncation of the series $F_\kappa(z) = \sum_{j=0}^{\infty} F_j(z)$ $(z < 0)$ of Theorem 2.11, as well as of the second given series expression for $F_j(z)$. Regarding the first given series expression for $F_j(z)$, the truncation error seems less easy to bound.

Proposition 3.4 *Let $z < 0$ and consider the series $F_\kappa(z) = \sum_{j=0}^{\infty} F_j(z)$ of Theorem 2.11. For all $J \in \mathbf{N}$ the truncation error is bounded by*

$$\left|\sum_{j=J}^{\infty} F_j(z)\right| < \sqrt{\frac{2|z|}{\pi}} \frac{1}{b\sqrt{1+b/|z|}} \binom{J-1/2}{J} \frac{\exp\left[b^2/|z| - b(4J+1)\right]}{1-\exp(-4b)}, \tag{3.5}$$

where b is any positive real number. Now consider the series in k in the second expression for $F_j(z)$. Provided that $K \geq j$, the truncation error satisfies
(3.6)
$$0 < \sum_{k=K}^{\infty} c(j,k) y^k D_{-k-3/2}\left(y(2j+3/2)\right) < e^{-y^2(j+1/2)} y^K D_{-K-3/2}(y(2j+1/2)),$$
where $y := \sqrt{2|z|}$ as in Theorem 2.11.

Note that, since $c(j,k) = 1$ for $k \geq j$, the upper error bound in (3.6) resembles $e^{-y^2(j+1/2)}$ times the K^{th} summand (first neglected summand), apart from a slightly changed argument of the parabolic cylinder function.

Regarding the bound for $\sum_{j=J}^{\infty} F_j(z)$, one has to choose a parameter value $b > 0$, the obvious aim being to make the bound strong (small). A good choice is

$$b := b(J,z) := |z| \left[J + 1/4 + \sqrt{(J+1/4)^2 + |z|^{-1}} \right]. \tag{3.7}$$

This b approximately minimises the bound in the sense that it exactly minimises the quantity $b^{-5/2} \exp[b^2/|z| - (4J+1)b]$ which results from the bound by replacing $1 - \exp(-4b)$ by its first order approximation $4b$ and dropping $\sqrt{1 + b/|z|}$ as well as all terms not containing b.

Proof. *Bound (3.5).* In order to bound $|F_j(z)|$ we write $F_j(z)$ in an integral form deduced from (2.25): after substituting $\sqrt{v} = w$,

$$F_j(z) = \sqrt{2} \binom{-1/2}{j} \frac{1}{\pi i} \int_{Q_\varepsilon} \frac{1}{w\sqrt{1 + w/|z|}} e^{w^2/|z| - (4j+1)w} \left(\frac{1 - w/|z|}{1 + w/|z|} \right)^j.$$

Here, the path Q_ε is the square root of the old path P_ε and hence goes from $e^{-\pi i/4}\infty$ to $e^{\pi i/4}\infty$ without encircling the singularities $w = 0$ and $w = -|z|$. Since the integrand is holomorphic on $\mathrm{Re}(w) > 0$, the path can be deformed to the straight line $(b - i\infty, b + i\infty)$ for any fixed $b > 0$. Along this new path we have $\mathrm{Re}(w) = b$, and hence we can bound

$$\begin{aligned}
|F_j(z)| &\leq \frac{\sqrt{2}}{\pi} \left| \binom{-1/2}{j} \right| \\
&\quad \int_{b-i\infty}^{b+i\infty} \left| \frac{1}{w\sqrt{1 + w/|z|}} e^{w^2/|z| - (4j+1)w} \left(\frac{1 - w/|z|}{1 + w/|z|} \right)^j \right| |dw| \\
&< \frac{\sqrt{2}}{\pi} \frac{1}{b\sqrt{1 + b/|z|}} \left| \binom{-1/2}{j} \right| e^{-(4j+1)b} \int_{b-i\infty}^{b+i\infty} e^{\mathrm{Re}(w^2)/|z|} |dw|.
\end{aligned}$$

By parameterizing,

$$\int_{b-i\infty}^{b+i\infty} e^{\mathrm{Re}(w^2)/|z|}\,|dw| = \int_{-\infty}^{\infty} e^{\mathrm{Re}((b+it)^2)/|z|}|i|dt$$
$$= e^{b^2/|z|}\int_{-\infty}^{\infty} e^{-t^2/|z|}dt = e^{b^2/|z|}\sqrt{|z|\pi},$$

and hence

$$|F_j(z)| < \sqrt{\frac{2|z|}{\pi}}\frac{1}{b\sqrt{1+b/|z|}}e^{b^2/|z|}\left|\binom{-1/2}{j}\right|e^{-(4j+1)b}.$$

So, by

$$\left|\sum_{j=J}^{\infty} F_j(z)\right| \leq \sum_{j=J}^{\infty}|F_j(z)|\,,$$

we deduce that

$$\left|\sum_{j=J}^{\infty} F_j(z)\right| < \sqrt{\frac{2|z|}{\pi}}\frac{1}{b\sqrt{1+b/|z|}}e^{b^2/|z|-b(4J+1)}\sum_{j=0}^{\infty}\left|\binom{-1/2}{j+J}\right|e^{-4bj}.$$

The claimed formula follows by noting that

$$\sum_{j=0}^{\infty}\left|\binom{-1/2}{j+J}\right|e^{-4bj} \leq \left|\binom{-1/2}{J}\right|\sum_{j=0}^{\infty}e^{-4bj} = \binom{J-1/2}{J}\left(1-e^{-4b}\right)^{-1}.$$

Bound (3.6). By $K \geq j$, in the truncation error we have $c(j,k) = 1$. Using an integral representation for the parabolic cylinder function (Gradshteyn and Ryzhik (1994), 1092, 9.241.2), we see that

$$0 < \sum_{k=K}^{\infty} c(j,k)y^k D_{-k-3/2}\left(y(2j+3/2)\right)$$
$$= e^{-y^2(2j+3/2)^2/4}\int_0^{\infty} e^{-ty(2j+3/2)-t^2/2}\sqrt{t}\sum_{k=K}^{\infty}\frac{y^k t^k}{\Gamma(k+3/2)}dt,$$

where we used the monotone convergence theorem to interchange summation and integration. Since

$$\sum_{k=K}^{\infty}\frac{y^k t^k}{\Gamma(k+3/2)} = y^K t^K\sum_{k=0}^{\infty}\frac{y^k t^k}{\Gamma(k+K+3/2)}$$
$$< \frac{y^K t^K}{\Gamma(K+3/2)}\sum_{k=0}^{\infty}\frac{y^k t^k}{k!} = \frac{y^K t^K e^{yt}}{\Gamma(K+3/2)},$$

we have

$$\begin{aligned}
&\sum_{k=K}^{\infty} c(j,k) y^k D_{-k-3/2}\left(y(2j+3/2)\right) \\
&< \frac{y^K}{\Gamma(K+3/2)} e^{-y^2(2j+3/2)^2/4} \int_0^\infty e^{-ty(2j+1/2)-t^2/2} t^{K+1/2} dt.
\end{aligned} \tag{3.8}$$

After writing $(2j+3/2)^2 = (2j+1/2)^2 + 4j + 2$ the claimed bound follows by again using the same integral representation of $D_p(\zeta)$. **QED**.

3.2.2 Case of $z > 0$: series truncation in Theorem 2.15

The expressions for $F_\kappa(z)$ of Theorem 2.15, which are valid when $z > 1/2$ and by conjecture also for $0 < z \leq 1/2$, have the form $F_\kappa(z) = -1 + \sum_{j=0}^\infty F_j(z)$ where the summand $F_j(z)$ is again written in two ways as series (in k). Unfortunately, the author is unable to derive an upper bound for $\left|\sum_{j=J}^\infty F_j(z)\right|$. A procedure similar to the case $z < 0$ seems impossible when $z > 0$.

Hence, while an "intuitive" truncation of $\sum_{j=0}^\infty F_j(z)$ is always possible, the author is unable to provide a mathematically well founded numerical approximation technique when $z > 0$.

Regarding the second series expression for the summand $F_j(z)$ in Theorem 2.15, with some technical effort a truncation error bound can be derived using an inequality satisfied by the parabolic cylinder function. However, without a truncation criterion for the outer series the error bound for the inner series is not of much use and is not reported here.

3.2.3 Case of $z < 0$: series truncation in Theorem 2.17

We now consider the expression of Theorem 2.17 which contains a single infinite series.

By Lemma 2.16 and after a substitution,

$$\begin{aligned}
F_j(z) &= 2(-z)^2 v \frac{1}{\pi i} \int_\Gamma g_j(z, 2(-z)^2 v^2) dv \\
&= \binom{j-1/2}{j} (-)^j \frac{\sqrt{2}}{\pi i} \int_\Gamma v^{-3/2} e^{-zv^2+zv} \left[v^{-1} + v^{-1} e^{4zv} - e^{4zv}\right]^j dv,
\end{aligned}$$

where Γ stands for the transformed path. By a triangle argument, Γ can be replaced by the old path $(b - i\infty, b + i\infty)$. Taking absolute values, we obtain

$$\left|\sum_{j=J}^{\infty} F_j(z)\right| \leq \sum_{j=J}^{\infty} |F_j(z)| < \sqrt{2}\sum_{j=J}^{\infty} \binom{j-1/2}{j} \int_{b-i\infty}^{b+i\infty} |v|^{-3/2}$$
$$e^{-z\,\mathrm{Re}(v^2)+zb} \left|v^{-1} + v^{-1}e^{4zv} - e^{4zv}\right|^j \frac{dv}{\pi i}.$$

So by the monotone convergence theorem,

$$\left|\sum_{j=J}^{\infty} F_j(z)\right| < \sqrt{2} \int_{b-i\infty}^{b+i\infty} |v|^{-3/2} e^{-z\,\mathrm{Re}(v^2)+zb}$$
$$\sum_{j=J}^{\infty} \binom{j-1/2}{j} \left|v^{-1} + v^{-1}e^{4zv} - e^{4zv}\right|^j \frac{dv}{\pi i}.$$

In this we have $|v| \geq b$ as well as

$$\begin{aligned}
&\sum_{j=J}^{\infty} \binom{j-1/2}{j} \left|v^{-1} + v^{-1}e^{4zv} - e^{4zv}\right|^j \\
&< \binom{J-1/2}{J} \sum_{j=J}^{\infty} \left(b^{-1} + b^{-1}e^{4zb} + e^{4zb}\right)^j \\
&= \binom{J-1/2}{J} \frac{\left(b^{-1} + b^{-1}e^{4zb} + e^{4zb}\right)^J}{1 - b^{-1} - b^{-1}e^{4zb} - e^{4zb}},
\end{aligned}$$

where the last step assumes that b is chosen large enough so that $b^{-1}+b^{-1}e^{4zb}+e^{4zb} < 1$. So,

$$\left|\sum_{j=J}^{\infty} F_j(z)\right| < \sqrt{2}b^{-3/2}e^{zb} \binom{J-1/2}{J} \frac{\left(b^{-1} + b^{-1}e^{4zb} + e^{4zb}\right)^J}{1 - b^{-1} - b^{-1}e^{4zb} - e^{4zb}}$$
$$\frac{1}{\pi i} \int_{b-i\infty}^{b+i\infty} e^{-z\,\mathrm{Re}(v^2)} dv.$$

Since

$$\frac{1}{\pi i} \int_{b-i\infty}^{b+i\infty} e^{-z\,\mathrm{Re}(v^2)} dv = \frac{1}{\pi} \int_{-\infty}^{\infty} e^{-z(b^2-y^2)} dy = \frac{1}{\sqrt{-z\pi}} e^{-zb^2},$$

we have proven the following bound:

Proposition 3.5 *Let $z < 0$ and $J \in \mathbf{N}$. For all $b > 0$ such that $b^{-1} + b^{-1}e^{4zb} + e^{4zb} < 1$, the truncation error $\sum_{j=J}^{\infty} F_j(z)$ satisfies*

$$\left|\sum_{j=J}^{\infty} F_j(z)\right| < \sqrt{\frac{2}{-z\pi}} \binom{J-1/2}{J} b^{-3/2} e^{-zb(b-1)} \frac{(b^{-1} + b^{-1}e^{4zb} + e^{4zb})^J}{1 - (b^{-1} + b^{-1}e^{4zb} + e^{4zb})}.$$

Determination of b

Our error bound depends on a parameter b. We now consider the determination of a "good" b (that makes the bound small). Let z and J be fixed and consider the bound as a function of b:

$$B(b) := B_J(z,b) := Ce^{-zb(b-1)} b^{-3/2} \frac{h(b)^J}{1-h(b)}, \tag{3.9}$$

where

$$C := C_J(z) := \sqrt{\frac{2}{-z\pi}} \binom{J-1/2}{J} \text{ and } h(b) := h(z,b) := b^{-1} + b^{-1}e^{4zb} + e^{4zb}.$$

Call a $b > 0$ "*admissible*" if $h(b) < 1$ (only then does the error bound hold). Since $h(b)$ is strictly decreasing in $b > 0$, the set of of admissible b's takes the form[1]

$$\{b \in \mathbf{R} | h(b) < 1\} = (b_0, \infty),$$

where $b_0 > 0$ is the unique positive solution of $h(b) = 1$.

We propose three ways of determining b.

1. A first, simple but perhaps not sufficiently efficient method is to choose an arbitrary admissible b, obtained by guessing a value b for which $B(b)$ is reasonably small and verifying that b is indeed admissible. Since $B(b) = B_J(z,b)$

---

[1] When looking for an admissible b for which $B(b)$ is small, then in the case that the value $b_1 := \left(1 + \sqrt{1 - 12/z}\right)/4$ is admissible ($h(b_1) < 1$), the search can be restricted to values b belonging to $[b_1, \infty)$. The reason is that $B(b)$ is strictly decreasing on $b \in (b_0, b_1)$. To see the latter, it is sufficient to show that in (3.9) the factor $b^{-3/2}e^{-zb(b-1)}$ is decreasing on (b_0, b_1) (the other factors being obviously strictly decreasing). Indeed,

$$\frac{d}{db} \ln\{b^{-3/2}e^{-zb(b-1)}\} = -\frac{3}{2}b^{-1} + z - 2zb,$$

which is negative for b between the two roots $(1 \pm \sqrt{1-12/z})/4$ of $-3/2 + zb - 2zb^2$, and hence in particular for $b \in (b_0, b_1)$.

has to be calculated for different J (until $B_J(z,b)$ is sufficiently small), b would either have to be newly chosen for each J, or chosen once for all J; in the latter case the choice of b has to suit many different J's, which is a difficult task given that one does not know in advance how large J has to become.

2. Another strategy is to determine b by using an available numerical minimisation tool. This strategy contains some difficulties such as the fact that the interval (b_0, ∞) of admissible b's is unknown since b_0 is unknown.

3. Given the disadvantages of the strategies 1 and 2, we now present our preferred procedure which is the search for a "good" b on an appropriate lattice.

By (3.9), on $b \in (b_0, \infty)$, the bound $B(b)$ equals C times the increasing function $\exp[-zb(b-1)]$ times a decreasing function. Obviously $B(b)$ tends to ∞ at both boundaries of (b_0, ∞), i.e. for $b \downarrow b_0$ and $b \to \infty$. From inspecting (3.9) it seems plausible that $B(b)$ is convex on (b_0, ∞), or at least that

$$\begin{gathered} B(b) \text{ has no local minimum on } (b_0, \infty) \\ \text{except a global minimum } b_m. \end{gathered} \tag{3.10}$$

In other words, (3.10) states that $B(b)$ is strictly decreasing on (b_0, b_m) and strictly increasing on (b_m, ∞). Unfortunately we are unable to prove (3.10). Plots of $B(b)$ for different values of z and J (with Maple 7) point at strict convexity of $B(b)$.[2] From now on we assume (3.10); if this assumption happened to be wrong for some combination of z and J, then the presented algorithm is likely to approximate the first local minimum (from the left) rather than the global minimum, and hence might still produce a reasonably good b. In any case, the calculated b is admissible.

We let b run from left to right through the lattice $\{n|z|^{-1/2}, n = 1, 2, ...\}$. After encountering the first admissible b the bound $B(b)$ is decreasing until it reaches its minimum on $\{n|z|^{-1/2}, n = 1, 2, ...\} \cap (b_0, \infty)$, from which on $B(b)$ is increasing. The minimizing value $\bar{b}$ can be obtained as:

$$\bar{b} := \bar{b}_J(z) := N|z|^{-1/2},$$

where

$$\begin{aligned} N := N_J(z) := \min\{n = 1, 2, ... | h(n|z|^{-1/2}) < 1 \\ \wedge\ B(n|z|^{-1/2}) < B((n+1)|z|^{-1/2})\}. \end{aligned} \tag{3.11}$$

[2]The strict convexity of the term $\exp[-zb(b-1)]$ on (b_0, ∞) can be shown by using that $b_0 > 1$.

In (3.11), the requirement $h(n|z|^{-1/2}) < 1$ ensures the admissibility of $\bar{b}$ and the requirement $B(n|z|^{-1/2}) < B((n+1)|z|^{-1/2})$ ensures that $\bar{b}$ is the "turning point" of $B(b)$ on the lattice. The step length of $|z|^{-1/2}$ is chosen so as to ensure that in $B(b)$ the argument of the exponential function, viz. $-zb(b-1) = |b|b^2 - |z|b$, does not vary strongly in one step, implying that $B(\bar{b})$ is reasonably close to $B(b_m)$.

For most if not all commonly needed pairs z, J the number $N_J(z)$ is small, barely exceeding 10, which is due to the very strong growth of the exponential function occurring in $B(b)$. Hence the computation of the bound $B(b)$ (including the determination of b as described) is efficient for most if not all relevant z, J.

If wished, an efficiency improvement in the calculation of $N_J(z)$ can be obtained by using that $N_{J-1}(z) \leq N_J(z)$ for all $z < 0$ and $J \geq 1$, which is because $B_J(z, b)$ equals $B_{J-1}(z, b)$ times a decreasing function of b. Hence, when calculating the bounds $B(\bar{b}_J(z))$ until reaching a J that makes the bound sufficiently small, the values $N_J(z)$ can be obtained recursively via:

$$
\begin{aligned}
N_0(z) &:= \min\{n = 1, 2, ... | h(n|z|^{-1/2}) < 1 \\
&\qquad\qquad\qquad \wedge\ B_0(z, n|z|^{-1/2}) < B_0(z, (n+1)|z|^{-1/2})\}, \\
N_J(z) &:= \min\{n \geq N_{J-1}(z) | B_J(z, n|z|^{-1/2}) < B_J(z, (n+1)|z|^{-1/2})\}
\end{aligned}
$$

where $J \geq 1$.

Chapter 4

Numerical Approximation

This chapter discusses the numerical approximation of values of $F_\tau(z)$ and $F_\kappa(z)$. Section 4.1 presents the general implementation recipe based on our truncation error bounds, including techniques to avoid numerical instability. Some additional advice is given in Section 4.2 where it is especially seen how many (expensive) evaluations of the incomplete gamma function in $F_\tau(z)$ or of the parabolic cylinder function in $F_\kappa(z)$ can be saved. The two last Sections 4.3 and 4.4 deal specifically with $F_\tau(z)$ respectively with $F_\kappa(z)$. Both sections contain large tables of highly accurate quantiles for the distribution of τ respectively κ, that were computed either with programs written in the elementary language Ox (cf. Doornik (1999)), or with Maple programs. Also, the convergence rates of the different series are discussed and compared. Overall, it is seen that in the case of $z < 0$ all formulae for $F_\tau(z)$ or $F_\kappa(z)$ allow an efficient and highly accurate approximation, apart when z is either very close to 0 or tends to $-\infty$. By contrast, the formulae for $F_\kappa(z)$ when $z > 0$ have very slowly converging series.

4.1 General implementation recipe

This section presents the concrete implementation technique for a numerical approximation of $F_\tau(z)$ and $F_\kappa(z)$. In the Sections 4.1.1 and 4.1.2 we discuss how truncation errors respectively machine rounding errors (including overflow) can be controlled, where the former uses the results of Chapter 3 and the latter uses standard numerical techniques.

Our notion of an (approximation) error is that of an absolute (not relative) error, and accordingly the precision of an approximation is the absolute precision (of course, the discussion can easily be translated into one using relative errors). Recall that in an approximation $\tilde{a} \in \mathbf{R}$ of $a \in \mathbf{R}$ the absolute error is $a - \tilde{a}$ and the relative error is $(\tilde{a} - a)/a$,[1] and the approximation has (absolute respectively relative) precision $p > 0$ if the (absolute respectively relative) error is at most p in absolute value.

Let F denote either of the distribution functions F_τ or F_κ and assume that, for some $z \in \mathbf{R}$, the value $F(z)$ should be approximated to some given (absolute) precision $p > 0$.

4.1.1 Controlling truncation errors

Each derived expression for F has essentially the form $F(z) = \sum_{j=0}^{\infty} F_j(z)$ and is valid only for $z < 0$ or only for $z > 0$. Consider first the expression of Theorem 2.17 for $F(z) = F_\kappa(z)$ $(z < 0)$ where $F_j(z)$ contains no second infinite summation. In this simple case, $F(z)$ should, obviously, be approximated by

$$\tilde{F}(z) := \sum_{j=0}^{J} F_j(z), \tag{4.1}$$

where the "*truncation order*" $J = J(z)$ is chosen to be the smallest integer ≥ -1 such that the bound for $\left|\sum_{j=J+1}^{\infty} F_j(z)\right|$ (given in Section 3.2.3) is $\leq p$.

Now consider any of the expressions in which $F_j(z)$ contains a second infinite series, say $F_j(z) = \sum_{k=0}^{\infty} F_{jk}(z)$. A numerical evaluation of $F(z)$ is based on choosing "*truncation orders*" $J := J(z)$ and $K_j := K_j(z)$, $j = 0, 1, ..., J$, all ≥ -1, and to approximate $F(z)$ by

$$\tilde{F}(z) := \sum_{j=0}^{J} \sum_{k=0}^{K_j} F_{jk}(z). \tag{4.2}$$

Both the outer and inner series truncations produce errors, respectively given by

$$\varepsilon(J) := \varepsilon(z, J) := \sum_{j=J+1}^{\infty} F_j(z)$$

and

$$\varepsilon_j(K_j) := \varepsilon_j(z, K_j) := \sum_{k=K_j+1}^{\infty} F_{jk}(z), \qquad j = 0, ..., J.$$

[1] Alternatively, one may define the absolute respctively relative errors as $\hat{a} - a$ respectively $(\hat{a} - a)/a$.

The sum of these errors gives the overall approximation error:

$$F(z) - \tilde{F}(z) = \varepsilon(J) + \sum_{j=0}^{J} \varepsilon_j(K_j). \tag{4.3}$$

From Chapter 3 we possess bounds for each truncation error, say $|\varepsilon(J)| \leq B(J)$ and $|\varepsilon_j(K_j)| \leq B_j(K_j)$, $j = 0, ..., J$. The truncation orders J and K_j, $j = 0, ..., J$, should be chosen such that

$$B(J) + \sum_{j=0}^{J} B_j(K_j) \leq p, \tag{4.4}$$

which implies $\left|F(z) - \tilde{F}(z)\right| \leq p$, as desired. There is some freedom in the way to achieve (4.4), corresponding to the different possible ways of decomposing the precision (or "distributing" the precision to the different series involved). A precision decomposition is given by these two steps:

1. p is decomposed into a sum $p = p' + p''$ ($p', p'' > 0$), and J is determined as the smallest integer ≥ -1 such that $B(J) \leq p'$.

2. p'' is decomposed into a sum $p'' = \sum_{j=0}^{J} p_j$ ($p_j > 0$, $j = 0, ..., J$), and K_j is determined as the smallest integer ≥ -1 such that $B_j(K_j) \leq p_j$, for all $j = 0, ..., J$.

In order to avoid having to compute many summands, the precision decomposition should be chosen such that a comparatively low precision is assigned to those series that have slow convergence. For instance, if the outer series $\sum_{j=0}^{\infty} F_j(z)$ has fast convergence and the inner series $\sum_{k=0}^{\infty} F_{jk}(z)$ has slow convergence for small j, then p' should be small, e.g. $p' = p/10$, and p_j should be large for small j, e.g. $p_j = 2^{-j}c$ where the factor c should be such that $\sum_{j=0}^{J} p_j$ indeed equals p'', viz. $p_j = 2^{-j-1}p''/(1 - 2^{-J-1})$. This precision decomposition is a suitable one for each of those expressions for $F_\tau(z)$ and $F_\kappa(z)$ valid for $z < 0$ and involving two series.

4.1.2 Controlling machine rounding errors and avoiding overflow

Besides truncation errors, a computer produces rounding errors in every operation. These may result in wrongly determined J and K_j, $j = 0, ..., J$ (because of imprecisely evaluated error bounds), and in imprecisely evaluated expressions

(4.1) respectively (4.2). To account for such errors, it is usually sufficient to give the computer a slightly lower value for p than the actually intended precision, for instance $p/2$ instead of p. The only danger[2] lays in the summations in (4.1) respectively (4.2): Arbitrarily high rounding errors can occur if individual summands become very large, while their sum is small due to varying signs. This case should be excluded as follows (we consider (4.1), the case of (4.2) being analogous). Note that, by Theorem 2.17, $F_j(z)$ in (4.1) is itself a finite sum, namely a sum of the form $F_j(z) = \sum_{k=0}^{j}\sum_{l=0}^{k} F_{jkl}(z)$ where $F_{jkl}(z)$ is now summation-free. Hence (4.1) becomes

$$\tilde{F}(z) = \sum_{j=0}^{J}\sum_{k=0}^{j}\sum_{l=0}^{k} F_{jkl}(z).$$

It has to be ensured that all terms $F_{jkl}(z)$ are sufficiently small. This is achieved by testing whether

$$\max\{|F_{jkl}(z)| : l = 0, ..., k \ \wedge \ k = 0, ..., j \ \wedge \ j = 0, ..., J\} \leq kp, \tag{4.5}$$

where $k > 0$ is a factor that should be chosen much smaller than 10^D where D denotes the number of floating-point digits that the software uses (for instance, $D = 32$); a possible choice is $k := 10^{D-10}$. If (4.5) failed to hold, then the only possible answer is to increase D. For instance, in Maple this is simply achieved by assigning the desired value D to the variable $Digits$.

Finally, overflow[3] should be excluded. If a series has to be truncated very late then, although all computed summands may stay moderate, some term in the summand, say z^k in a series in k, may become irrepresentable since z^k tends to 0 when $|z| < 1$, respectively to ∞ (in absolute value) when $|z| > 1$. This problem may occur (for certain $z < 0$) in the Leibniz series $\sum_{k=0}^{\infty} F_{jk}(z)$ in Theorem 2.22, when $j = 0$ and the required precision p is high. The problem can often be avoided by using logarithms: for instance if $z > 1$ then $z^k/k!$ should be programmed as $\exp[k\log(z) - \log\Gamma(k+1)]$, where $\log\Gamma$ is the log-gamma function. In the case that such techniques are not possible, one should use software that allows virtually unbounded exponents in floating-point arithmetics, such as Maple.

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[2] Numerical instability may also result from recurrence relations if these are used; see Section 4.2.1 and Appendix F.

[3] In a floating point representation, the exponent is restricted to some range, for instance -400 to $+400$, and overflow typically occurs when a term in an expression is too small or too large in absolute value.

4.2 Efficiency improvements and some related advice

This section gives some additional advice on programming the formulae, in particular in order to improve the efficiency. Section 4.2.1 discusses the use of updating relations. Section 4.2.2 mentions how the parabolic cylinder function can be expressed in terms of modified Bessel functions: the latter functions are more commonly included in program libraries than the former. Section 4.2.3 discusses how to avoid multiple evaluations of the occurring higher transcendental functions, in particular through sum reorderings.

4.2.1 Using updating relations

As is discussed in more detail in Appendix F, a common programming technique is the use of recurrence (or *updating*) relations in order to avoid costly new evaluations. This applies in particular to the incomplete gamma functions occurring in $F_\tau(z)$ and to the parabolic cylinder functions occurring in $F_\kappa(z)$ and in some error bounds. The following updating relations can be used:

$$\begin{aligned} &\Gamma(p+1,\zeta) - p\Gamma(p,\zeta) - \zeta^p e^{-\zeta} = 0, \\ &D_{p+1}(\zeta) - \zeta D_p(\zeta) + pD_{p-1}(\zeta) = 0, \end{aligned} \tag{4.6}$$

cf. Gradshteyn and Ryzhik (1994), p. 951, 8.356 and p. 1094, 9.247. Since the incomplete gamma function enters the formulae for $F_\tau(z)$ as terms of the form $\Gamma(1/4+n/2,\zeta)$ with integer n, one might "directly" evaluate only $\Gamma(1/4,\zeta)$ and $\Gamma(-1/4,\zeta)$ and calculate all other needed $\Gamma(1/4+n/2,\zeta)$ by recursion. Analogously, the expressions for $F_\kappa(z)$ contain terms of the form $D_{n-1/2}(\zeta)$ with integer n, and one might "directly" calculate only $D_{-1/2}(\zeta)$ and $D_{1/2}(\zeta)$, while using the recurrence relation for all other needed terms $D_{n-1/2}(\zeta)$.

Appendix F discusses how to prevent the danger of possible accumulation of large rounding errors due to numerical instability in the badly conditioned[4] addition in these updating relations. Appendix F shows how to test the magnitude of rounding errors; if this test reveals too large errors, it is necessary to work with a higher floating point precision.

[4] The sum of two quantities each containing small relative errors has a large relative error if the summands are similar in absolute value but of opposite sign.

4.2.2 Avoiding the parabolic cylinder function

Many program libraries do not contain the parabolic cylinder function $D_p(\zeta)$. Luckily, in our special case where p has the form $p = n - 1/2$ with integer n, the function $D_{n-1/2}(\zeta)$ can (for $\zeta > 0$) be expressed as a linear combination of $|n| + 1$ modified Bessel functions, e.g.:

$$
\begin{aligned}
D_{-1/2}(\zeta) &= \frac{b}{\sqrt{\pi}} K_{1/4}, \\
D_{1/2}(\zeta) &= \frac{b^3}{\sqrt{\pi}} (K_{1/4} + K_{3/4}), \\
D_{-3/2}(\zeta) &= \frac{2b^3}{\sqrt{\pi}} (-K_{1/4} + K_{3/4}), \\
D_{3/2}(\zeta) &= \frac{b^5}{\sqrt{\pi}} (2K_{1/4} + 3K_{3/4} - K_{5/4}), \\
D_{-5/2}(\zeta) &= \frac{4b^5}{3\sqrt{\pi}} (2K_{1/4} - 3K_{3/4} + K_{5/4}),
\end{aligned} \tag{4.7}
$$

where $b := \sqrt{\zeta/2}$ and the omitted argument of all modified Bessel functions K_p (cf. Appendix A) is $\zeta^2/4$, i.e. $K_p := K_p(\zeta^2/4)$ (Magnus and Oberhettinger, 1966, p. 326). So, one might use this representation in order to calculate $D_{-1/2}(\zeta)$ and $D_{1/2}(\zeta)$ and then use the recursion relation for all other needed $D_{n-1/2}(\zeta)$.

4.2.3 Avoiding multiple evaluations

For most of the formulae for $F_\tau(z)$ respectively $F_\kappa(z)$, "naive" programming leads to multiple evaluation of the same term $\Gamma(p, \zeta)$ respectively of the same term $D_p(\zeta)$. For instance, $\Gamma(1/4 - l/2 + k/2, \zeta)$ is the same for $l = k = 0$ and $l = k = 1$. In order to avoid multiple evaluation, one can either store the relevant quantities in an array to be recalled later, or, perhaps more elegantly, by reordering summations. This latter strategy is below discussed for the different formulae.

The expressions for $F_\tau(z)$.

Theorem 2.22 (valid for $z < 0$) gives two expressions for $F_\tau(z)$, each containing two infinite and one finite sum. Truncation of the infinite series yields corresponding approximations of $F_\tau(z)$, viz.

$$F_\tau(z) \approx \begin{cases} \sqrt{\frac{x}{\pi}} e^{-x^2/4} \sum_{j=0}^{J} \binom{j-1/2}{j} \sum_{k=0}^{K} \sum_{l=0}^{j} F_{j,k,l}(z), & x := 2^{1/2}|z|, \\ \sqrt{\frac{2y}{\pi}} \sum_{j=0}^{J} \binom{j-1/2}{j} \sum_{k=0}^{K} \sum_{l=0}^{j} F_{j,k,l}(z), & y := 2^{-1/2}|z|, \end{cases}$$

where $F_{j,k,l}(z)$ is different in form and value in both formulae and K may depend on j and z. In the first respectively second formula $F_{j,k,l}(z)$ contains $\Gamma(1/4 - l/2 + k/2, \zeta)$ respectively $\Gamma(1/4 - l/2 - k/2, \zeta)$ (with $\zeta = \zeta(z, j)$ independent of k and l, but different in both formulae). This term depends on k and l only through $k - l$ respectively through $k + l$, and multiple evaluations can be avoided by reordering the double sum $\sum_{k=0}^{K} \sum_{l=0}^{k} F_{j,k,l}(z)$. In the case of the second formula, however, a sum reordering is not advisable and the technique of saving in an array should be preferred: Indeed, the sum in k is a Leibniz series, and the convenient truncation criterion[5] would not be usable in a reordered sum.

So, let us consider the first approximation formula. By introducing the parameter $m = k - l$ we can reorder as follows:

$$\sum_{k=0}^{K} \sum_{l=0}^{j} F_{j,k,l}(z) = \sum_{k=0}^{K} \sum_{m=k-j}^{k} F_{j,k,k-m}(z) = \sum_{m=-j}^{K} \sum_{k=\max\{0,m\}}^{\min\{K,m+j\}} F_{j,k,k-m}(z),$$

which by the particular form of $F_{j,k,l}(z)$ equals

$$\sum_{m=-j}^{K} (-)^m \Gamma\left(\frac{1}{4} + \frac{m}{2}, x^2(2j+1)^2\right) \sum_{k=\max\{0,m\}}^{\min\{K,m+j\}} \frac{(-)^k}{k!} \binom{j}{k-m} x^{2k-m}.$$

The two-series expression for $F_\kappa(z)$.

Now consider the formulae for $F_\kappa(z)$ containing two infinite series. The Theorems 2.11 and 2.15 are valid for the cases $z < 0$ respectively $z > 0$ and each provide two such expressions for $F_\kappa(z)$. An advantage of the second expression of each theorem is that they need no sum reordering: indeed, programming of these formulae as such leads to no multiple evaluation of the parabolic cylinder function.

[5] The Leibniz series in k should be truncated as soon as the summand, viz. $\sum_{l=0}^{j} F_{j,k.l}(z)$, is smaller in absoluted value than the required precision.

By contrast, consider the first formula of each Theorem. Truncation of both series (in j respectively k) leads to approximations of the kind

$$F_\kappa(z) \approx \begin{cases} 2\sqrt{\frac{y}{\pi}} \sum_{j=0}^{J} \binom{j-1/2}{j} e^{-y^2(j^2-j/2+7/16)} \sum_{k=0}^{K} \sum_{l=0}^{j} F_{j,k,l}(z), & z<0, \\ -1+\sqrt{8y} \sum_{j=0}^{J} \binom{j-1/2}{j} e^{y^2(j^2-j/2-7/16)} \sum_{k=0}^{K} \sum_{l=0}^{j} F_{j,k,l}(z), & z>0, \end{cases}$$

with $F_{j,k,l}(z)$ different in form depending of the sign of z, and where J may depend on z and K may depend on j and z. The summand $F_{j,k,l}(z)$ contains a parabolic cylinder function that depends on k and l only through $k+l$. Multiple evaluations can be avoided by reordering the double sum $\sum_{k=0}^{K} \sum_{l=0}^{j} F_{j,k,l}(z)$ according to:

$$\sum_{k=0}^{K} \sum_{l=0}^{j} F_{j,k,l}(z) = \sum_{k=0}^{K} \sum_{m=k}^{j+k} F_{j,k,m-k}(z) = \sum_{m=0}^{j+K} \sum_{k=\max\{0,m-j\}}^{\min\{K,m\}} F_{j,k,m-k}(z).$$

Given the particular form of $F_{j,k,l}(z)$ this leads to

$$\sum_{k=0}^{K} \sum_{l=0}^{j} F_{j,k,l}(z)$$
$$= \begin{cases} \sum_{m=0}^{j+K} e_K(j,m) y^m D_{-m-3/2}\left(y(2j+3/2)\right), & z<0, \\ \sum_{m=0}^{j+K} e_K(j,m) y^m D_{m+1/2}\left(y(2j+3/2)\right)/\Gamma(m+3/2), & z>0, \end{cases}$$

where again $y := \sqrt{2|z|}$, and where we have put

$$e_K(j,m) := \sum_{k=\max\{0,m-j\}}^{\min\{K,m\}} \binom{j}{m-k} (-2)^{m-k} = \sum_{k=m-\min\{K,m\}}^{m-\max\{0,m-j\}} \binom{j}{k} (-2)^k.$$

The one-series expression for $F_\kappa(z)$.

In Theorem 2.17 $F_\kappa(z)$ is for negative z expressed as a series $F_\kappa(z) = \sum_{j=0}^{\infty} F_j(z)$ where $F_j(z)$ is composed of two finite summations: say, $F_j(z) = \sum_{k=0}^{j} \sum_{l=0}^{k} F_{j,k,l}(z)$ with $F_{j,k,l}(z)$ containing the parabolic cylinder function $D_{-k-3/2}(2(j+l-k+1/4)y)$. Hence an approximation $F_\kappa(z) \approx \sum_{j=0}^{J} F_j(z)$ necessitates the evaluation of $O(J^3)$ summands $F_{j,k,l}(z)$. However, by avoiding multiple evaluations through a sum reordering, it can be ensured that the parabolic cylinder function $F_{j,k,l}(z)$ is evaluated only $O(J^2)$ times. This is not surprising because $D_{-k-3/2}(2(j+l-k+1/4)y)$ depends on j and l only through $j+l$, so that it should suffice to evaluate $D_{-k-3/2}(2(m+1/4)y)$ for all $k,m=0,...,J$, hence $(J+1)^2=O(J^2)$ times. We now reparametrise the summations by introducing the parameter $m=j+l-k$:

$$\begin{aligned}\sum_{j=0}^{J} F_j(z) &= \sum_{j=0}^{J}\sum_{k=0}^{j}\sum_{l=0}^{k} F_{j,k,l}(z)\\ &= \sum_{j=0}^{J}\sum_{k=0}^{j}\sum_{m=j-k}^{j} F_{j,k,m+k-j}(z) = \sum_{m=0}^{J}\sum_{k=0}^{J}\sum_{j=\max\{k,m\}}^{\min\{k+m,J\}} F_{j,k,m+k-j}(z).\end{aligned}$$

Given the particular form of $F_{j,k,l}(z)$ we can code $\sum_{j=0}^{J} F_j(z)$ more efficiently as

$$\begin{aligned}\sum_{j=0}^{J} F_j(z) = 2\sqrt{\frac{y}{\pi}}&\sum_{m=0}^{J}\exp(-(m+1/4)^2y^2)\\ &\times\sum_{k=0}^{J}(-y)^k d_J(k,m) D_{-k-3/2}(2(m+1/4)y),\end{aligned}$$

with coefficient

$$\begin{aligned}d_J(k,m) :=& \sum_{j=\max\{k,m\}}^{\min\{k+m,J\}}\binom{j-1/2}{j}\binom{j}{k}\binom{k}{m+k-j}\\ =& \sum_{j=\max\{k,m\}}^{\min\{k+m,J\}}\frac{(1/2)_j}{(j-k)!(j-m)!(k+m-j)!}.\end{aligned}$$

Note that the computation of the values $d_J(k,m)$, $k,m=0,...,J$, can be speeded up by using the symmetry $d_J(k,m)=d_J(m,k)$.

4.3 Approximation for the t statistic

In this section, let $z<0$. Both expressions of Theorem 2.22 permit an efficient and accurate computation of values $F_\tau(z)$ for all commonly used negative quantiles z. After reporting a table of quantiles, we give a detailed numerical discussion. While the new series in k (2.51) has a particularly comfortable truncation criterion (due to the Leibniz property), it is seen that Abadir's series in k (2.50) has a faster convergence for $j = 0$ and most z.

Table of quantiles

The Table 4.1 of quantiles for τ was computed using Abadir's expression, and some correctness tests were done by comparing with the new expression.

α	α-quantile	α	α-quantile
65%	-.0981	4.0%	-2.0366
60%	-.2402	3.5%	-2.0922
55%	-.3743	3.0%	-2.1550
50%	-.5001	2.5%	-2.2274
45%	-.6180	2.0%	-2.31353
40%	-.73156	1.5%	-2.42086
35%	-.84535	1.0%	-2.56580
30%	-.96373	.75%	-2.66464
25%	-1.09127	.50%	-2.79893
20%	-1.23403	.25%	-3.01661
15%	-1.40215	.10%	-3.28511
10%	-1.6167	.075%	-3.36553
9%	-1.66903	.050%	-3.47608
8%	-1.7261	.025%	-3.65817
7%	-1.78914	.010%	-3.8871
6%	-1.85984	.005%	-4.0525
5%	-1.94087	.001%	-4.4147
4.5%	-1.98652		

Table 4.1: Quantiles of τ

The quantiles are accurate in the following two senses:

(a) Each reported digit is correct (in the sense of rounding rather than truncating).

(b) If q_α is the (exact) α-quantile and $\hat{q}_\alpha$ is the value reported, then $F_\tau(\hat{q}_\alpha)$ approximates α to a *relative* error of less than 10^{-4}, i.e. $|F_\tau(\hat{q}_\alpha) - \alpha| / \alpha < 10^{-4}$.

The numbers of reported digits for quantiles vary and were chosen so as to guarantee (b). Note that up to 6 digits are necessary although (b) does not seem an excessive accuracy requirement.

In the literature, very low quantiles such as the 0.01%-quantile are rarely or never reported due to the difficulty of simulating low quantiles. Also, our table is more accurate than any such table in the literature. For instance, Hamilton (1994, p. 763) reports the 5%-quantile as -1.95 and the 1%-quantile as -2.58; not only is the last digit of both figures wrong (violating (a)), but also (b) is violated because $F_\tau(-1.95) \approx 4.9\%$ and $F_\tau(-2.58) \approx 0.96\%$.

The outer series

Consider first the (outer) series in j of Theorem 2.22, $F_\tau(z) = \sum_{j=0}^\infty F_j(z)$, and the determination of the truncation order $J(z)$ based on the error bound (3.1), as discussed in Section 4.1.1. As $J \to \infty$ the bound (3.1) is of smaller order than $O\{\exp(-z^2(4J+1)^2/2)\}$, confirming the remark of Abadir (1995, p. 789) of an extremely rapid convergence of the outer sum. For instance if $z = -1$, then we have the following error bounds:

$$\sum_{j=1}^\infty F_j(-1) < .189 \cdot 10^{-6}, \quad \sum_{j=2}^\infty F_j(-1) < .404 \cdot 10^{-19}, \tag{4.8}$$

so that for $z = -1$ the first summand $F_0(z)$ on its own is already a very precise approximation of $F_\tau(z)$, and is an even better one if $z < -1$ since the bound (3.1) is increasing in z. Since $F_\tau(-1) \approx 29\%$, all commonly used quantiles for testing $\alpha = 1$ against $\alpha < 1$ satisfy $z < -1$. Thus, in practice, in the region of the common quantiles one can calculate $F_\tau(z)$ by dropping the outer sum: $F_\tau(z) \approx F_0(z)$. Notice how the two expressions (2.50) and (2.51) for $F_j(z)$ simplify if $j = 0$:

$$F_0(z) = \sqrt{\frac{x}{\pi}} e^{-x^2/4} \sum_{k=0}^\infty \frac{x^k}{k!} \Gamma\left(\frac{1}{4} + \frac{k}{2}, x^2\right), \quad x := 2^{1/2}|z| > 0, \tag{4.9}$$

$$= \sqrt{\frac{2y}{\pi}} \sum_{k=0}^\infty \binom{-1/2}{k} y^k \Gamma\left(\frac{1}{4} - \frac{k}{2}, y^2\right), \quad y := 2^{-1/2}|z| > 0. \tag{4.10}$$

Higher quantiles up to the 68%-quantile belong to the interval $-1 \leq z < 0$. Table 4.2 gives for different z the smallest integer $J \geq -1$ for which our bound for the error $(0 <)\ \varepsilon := \varepsilon(J) := \sum_{j=J+1}^\infty F_j(z)$, and hence ε itself, is smaller than 10^{-n} for different n.

	$z=-5$	$z=-1$	$z=-.5$	$z=-.1$	$z=-.05$	$z=-.01$
$\varepsilon < 10^{-4}$	-1	0	1	7	15	76
$\varepsilon < 10^{-8}$	0	1	2	12	25	124
$\varepsilon < 10^{-16}$	0	1	3	19	38	192
$\varepsilon < 10^{-32}$	0	2	5	28	57	285

Table 4.2: Truncation Orders for the outer series in F_τ

Table 4.2 should be used as follows. If, for any given $z \leq -0.01$, the truncation error $\varepsilon(J)$ should be smaller than 10^{-n}, where $n \in \{4, 8, 16, 32\}$, then choose J to be as given by the table for the *next higher* z. For instance, if $z = -0.3$ the choice of $J = 7$ guarantees that $\varepsilon(J) < 10^{-4}$.

Abadir's inner series

If the parabolic cylinder function is provided by the software, Abadir's series in k can be truncated using the error bound (3.2). This approximation is most efficient[6] and accurate, since the number of needed summands is small or moderate for all commonly used negative z (say for $z \in [-4, 0)$), even for very high required precision such as $p = 10^{-20}$.

If the parabolic cylinder function is not available, the weaker bound of Corollary 3.3 can be used which, however, becomes inefficient if z gets far from 0: one needs several hundred summands near the 5%-quantile, over thousand summands near the 2.5%-quantile, and over ten-thousand summands near the 1%-quantile, even at low standards of accuracy.

Note further that it may be worthwhile to avoid multiple evaluations of the same bound for different j; indeed, both presented bounds for the series in k are independent of j.

In analogy to Table 4.2, the Table 4.3 gives for different z the smallest integer[7] $K \geq 0$ for which our bound for the error[8] $(0 <)\ e_j := e_j(K) :=$

---

[6] It may, however, be that the computation of the parabolic cylinder function becomes slow for certain needed arguments (such as in Maple). Then, it is advisable to either use the recurrence relation (4.6), or to compute and test the bound only for certain K, say for $K = 30n$, $n = 1, 2, ..$; in the latter case, fewer bounds, but more summands $F_j(z)$ have to be computed, which may improve the overall efficiency.

[7] K may not be -1: the series can be truncated at the earliest after the first summand because Proposition 3.1 does not provide a bound for $\sum_{k=0}^{\infty} \delta_{jk}(z)$.

[8] $e_j(K)$ should be distinguished from $\varepsilon_j(K) := \sum_{j=K+1}^{\infty} F_{jk}(z)$. The summand $F_{jk}(z)$ comes from the representation $F_j(z) = \sum_{k=0}^{\infty} F_{jk}(z)$; since $F_j(z) = \sqrt{\frac{x}{\pi}} e^{-x^2/4} \binom{j-1/2}{j} \sum_{k=0}^{\infty} \delta_{jk}(z)$, we have $F_{jk}(z) = \sqrt{\frac{x}{\pi}} e^{-x^2/4} \binom{j-1/2}{j} \delta_{jk}(z)$.

$\sum_{k=K+1}^{\infty} \delta_{jk}(z)$, and hence e_j itself, is smaller than 10^{-n} for different n. Note that these K are independent of j since so is the bound (3.2).

	$z=-12$	$z=-6$	$z=-3$	$z=-1$	$z=-.1$	$z=-.001$
$e_j < 10^{-4}$	938	240	66	13	3	1
$e_j < 10^{-8}$	950	252	76	20	6	2
$e_j < 10^{-16}$	974	274	95	32	11	4
$e_j < 10^{-32}$	1022	316	128	52	21	9

Table 4.3: Truncation Orders for Abadir's inner series in F_τ

As Table 4.2, this table does not only bear information about those z mentioned in the table. Indeed, for any given $-12 < z < 0$ not mentioned, choose the *next smaller* z reported by the table, and the inequalities that hold for this z all the more hold for the larger z. The reason is that the bound (3.2) is decreasing in z. For instance, if $z = -2$ then $K = 76$ suffices for a precision of 10^{-8}.

The new inner series

Now let $\sum_{k=0}^{\infty} F_{jk}(z)$ be the Leibniz series (2.51) for $F_j(z)$. This series converges for $j \geq 1$ very fast and much faster than for $j = 0$. So, in order to avoid too many summands in the approximation of $F_0(z)$, the "precision decomposition" (cf. Section 4.1.1) should ask a comparatively low precision (called p_0 in Section 4.1.1) from $\sum_{k=0}^{\infty} F_{jk}(z)$ when $j = 0$.

Using the Leibniz series (and a suitable precision decomposition), a table of all values $F_\tau(z)$ on $z \in [-5, -0.01] \cap \{n/100 : n \in \mathbf{Z}\}$ can be computed within seconds[9], provided that the required precision is limited to $p = 10^{-4}$.

Now suppose that a higher precision than $p = 10^{-4}$ is required. Then the computation of a single value $F_\tau(z)$ can take seconds, due to an exploding number of needed summands from the series $F_0(z) = \sum_{k=0}^{\infty} F_{0k}(z)$. Moreover, overflow in the summands $F_{0k}(z)$ has to be prevented with the techniques mentioned in Section 4.1.2: indeed, if $k \to \infty$, then in $F_{0k}(z)$ one of the terms y^k and $\Gamma(1/4 - k/2, y^2)$ tends to $+\infty$ and the other one to 0, depending on whether $y = 2^{-1/2}|z|$ is greater or smaller than 1.

Note that in the Leibniz series, the truncation order $K_j(z)$ needed to reach a given precision is not a monotone function of z, but increases and decreases on different intervals for z. Hence a table analogous to the above tables (4.2) and

[9] This was done on an ordinary personal computer and using the elementary programing language "Ox", version 2.20 (Doornik, 1999).

(4.3) would be of little use, since it bears no information for a z not contained in the table. Besides, $K_j(z)$ depends on j, so that a whole collection of tables would be needed.

Extreme values of z
Problems of efficiency can arise for extreme values of z:

- If $z \uparrow 0$, the number of summands needed from the series in j is exploding, as can be seen from the bound (3.1). Luckily, for both Abadir's and the new inner series the number of summands needed to approximate each $F_j(z)$ becomes very small as $z \uparrow 0$, so that an accurate approximation of $F_\tau(z)$ is efficiently possible at least until $z = -0.01$.

- Let $z \to -\infty$ (at least $z < -5$) and suppose that the required precision is high enough to ensure $J(z) > -1$ (i.e. at least the first summand $F_0(z)$ is needed).[10] Given this very high required precision, Abadir's inner series is preferable to the Leibniz series. The number $K_0(z)$ needed to approximate $F_0(z)$ explodes as $z \to -\infty$, so that an efficient approximation finally fails. In fact, as can be seen from (4.9), for large $|z|$ the summands in $F_0(z) = \sum_{k=0}^{\infty} F_{0k}(z)$ start very small and increase until a certain k, before finally starting to converge towards 0, the turning point k occurring very late for very large $|z|$.

4.4 Approximation for the normalised coefficient estimator

This section discusses the specific numerical properties of different series expressions derived for $F_\kappa(z)$. We treat the case $z < 0$ (cf. Section 4.4.1), the case $z > 0$ (cf. Section 4.4.2), and the case $z < 0$ based on the expression involving a single infinite summation (cf. Section 4.4.3). For $z < 0$, either formula is seen to allow an accurate and efficient approximation of $F_\kappa(z)$, except for $z \uparrow 0$ or $z \to -\infty$. Section 4.4.4 compares the performance of both formulae when $z \uparrow 0$ or $z \to -\infty$.

[10]Such a situation can for instance arise when $F_\tau(z)$ should have a certain *relative* precision: As $z \to -\infty$, the corresponding required *absolute* precision p tends to 0 since $\lim_{z\to-\infty} F_\tau(z) = 0$.

4.4.1 Case of $z < 0$: numerical implementation of Theorem 2.11

As done earlier for the t statistic (cf. Section 4.3), we report a table of quantiles for κ, followed by a detailed numerical discussion for the outer and the inner series in $F_\kappa(z)$. The relevant expression for $F_\kappa(z)$ and truncation error bounds were given in Theorem 2.11 respectively Proposition 3.4.

Table of quantiles

The table of quantiles below for κ was obtained identically for the two-series expression (Theorem 2.11) and the later discussed one-series expression (Theorem 2.17).

α	α-quantile	α	α-quantile
65%	-.1376	4.0%	-8.805
60%	-.3591	3.5%	-9.2668
55%	-.5960	3.0%	-9.8027
50%	-.8528	2.5%	-10.4403
45%	-1.1380	2.0%	-11.2256
40%	-1.4618	1.5%	-12.2454
35%	-1.8370	1.0%	-13.6954
30%	-2.2812	.75%	-14.732
25%	-2.8209	.50%	-16.2026
20%	-3.5002	.25%	-18.7392
15%	-4.4020	.10%	-22.128
10%	-5.7137	.075%	-23.1989
9%	-6.061	.050%	-24.713
8%	-6.4523	.025%	-27.3136
7%	-6.899	.010%	-30.771
6%	-7.419	.005%	-33.3992
5%	-8.0391	.001%	-39.5358
4.5%	-8.3999		

Table 4.4: Quantiles of κ

As with table (4.1) for τ, this table satisfies the following two accuracy requirements:

(a) Each reported digit is correct (in the sense of rounding rather than truncating).

(b) If q_α is the (exact) α-quantile and $\hat{q}_\alpha$ is the value reported, then $F_\tau(\hat{q}_\alpha)$ approximates α to a *relative* error of less than 10^{-4}, i.e. $|F_\tau(\hat{q}_\alpha) - \alpha| / \alpha < 10^{-4}$.

As with the t statistic, between 4 and 6 digits are necessary to satisfy (b).

Again, simulation based tables often contain inaccuracies and do not cover very low quantiles due to the difficulty of simulating low quantiles. Hamilton (1994, p. 762) reports the 5%-quantile as -8.1, the 2.5%-quantile as -10.5, and the 1%-quantile as -13.8; (a) is violated because the last digit is wrong each time, and (b) is violated because $F_\kappa(-8.1) \approx 4.9\%$, $F_\kappa(-10.5) \approx 2.46\%$ and $F_\kappa(-13.8) \approx 0.97\%$.

The outer series

Our error bound (*3.5*) (with the parameter b given by (3.7)) is accurate for most z, thereby avoiding the evaluation of many unnecessary summands $F_j(z)$. Much as with the t statistic, it turns out that the series in j has a very fast convergence, unless z is close 0. For instance,

$$\sum_{j=1}^{\infty} F_j(-2) < 0.219 \times 10^{-6}, \quad \sum_{j=2}^{\infty} F_j(-2) < .512 \times 10^{-19}, \tag{4.11}$$

so that $F_\kappa(-2)$ is very well approximated by $F_0(-2)$ alone. Unfortunately, we are unable to prove the monotone growth in $z < 0$ of the error bound, although plausible and confirmed by plots with Maple 7. If the monotone growth holds, then by (4.11) we have the accurate approximation $F_\tau(z) \approx F_0(z)$ for all $z \leq -2$ and hence in particular in the region of the common low quantiles quantiles (1%, 2.5%, 5%, 10%). Note that when $j = 0$ the two expressions of Theorem 2.11 for $F_j(z)$ simplify to the same series, viz.:

$$F_0(z) = 2\sqrt{\frac{y}{\pi}} e^{7y^2/16} \sum_{k=0}^{\infty} y^k D_{-k-3/2}(3y/2).$$

In analogy to Table 4.2, the below Table 4.5 gives for different z the smallest integer $J \geq -1$ for which our bound for the error $\varepsilon := \varepsilon(J) := \sum_{j=J+1}^{\infty} F_j(z)$, and hence ε itself, is strictly bounded by 10^{-n} for different n.

	$z = -50$	$z = -5$	$z = -1$	$z = -.1$	$z = -.01$	$z = -.001$
$\lvert\varepsilon\rvert < 10^{-4}$	-1	0	1	3	11	34
$\lvert\varepsilon\rvert < 10^{-8}$	0	0	1	5	17	56
$\lvert\varepsilon\rvert < 10^{-16}$	0	1	2	8	27	86
$\lvert\varepsilon\rvert < 10^{-32}$	0	1	3	12	40	128

Table 4.5: Truncation orders for the outer series in F_κ

If it was believed that the error bound is indeed a growing function in $z \in \mathbf{R}_-$, then this table could again be used for any given $z \leq -.001$ by referring to the *next higher* z mentioned by the table.

The inner series

Since we possess a truncation error bound only for the second inner series of Theorem 2.11, this (rather than Abadir's) inner series should be used to calculate $F_j(z)$. Further advantages of the second expressions are that the finite sum in l is restricted to the coefficient $c(j,k)$ and does not contain the parabolic cylinder function; hence, expensive multiple evaluations of the latter need not be excluded by a sum reordering (cf. Section 4.2.3); further, if the coefficient $c(j,k)$ is calculated using the expression (2.32)-(2.33), any numerical instability or overflow can be avoided (even for very large j,k) since (2.32)-(2.33) is a sum of terms that all have the same sign (by contrast, the sum (2.30)-(2.31) for $c(j,k)$ should not be used since it is alternating, and individual terms can become much larger than their sum, possibly leading to instability).

So, let $F_j(z) = \sum_{k=0}^{\infty} F_{jk}(z)$ be the second series of Theorem 2.11. For all relevant z, this series converges quite fast, and the truncation order $K_j(z)$ usually is far below 100, even at high required precision[11]. However, since our error bound for $\sum_{k=K}^{\infty} F_{jk}(z)$ only holds when $K \geq j$, at least the summands $F_{j0}(z), ..., F_{j,j-1}(z)$ have to be evaluated. Hence, if J is the truncation order for the outer series, then in total at least $\sum_{j=0}^{J}\sum_{k=0}^{j-1} 1 = J(J+1)/2 = O(J^2)$ summands have to be evaluated. This leads to an efficiency problem only for z very close 0 where J becomes large.

[11] We assume a straightfroward decomposition of precision (cf. section 4.1), such as $p' = p''$ and $p_j = p''/(J+1)$.

A (possibly not worthwhile) efficiency improvement is achieved by using the fact that the bound for $\sum_{k=K}^{\infty} F_{jk}(z)$ is decreasing[12] as a function of $j(\leq K)$: After choosing a precision decomposition (cf. Section 4.1.1) satisfying $p_j = p_0$ for $j = 1, ..., J$, and evaluating the truncation order K_j for $j = 0$, one may put $K_j := K_0$ for all j satisfying $j \leq K_0$ (if $j > K_0$ this choice of K_j is not allowed because K_j has to be at least j, as mentioned earlier). By this method, K_j is possibly larger than necessary, but some bound evaluations may have been saved.

Note that our bound is not monotone in z, implying that the number K_j needed to reach a given precision of the inner series is not a monotone function of z. So, as with the Leibniz series in Section 4.3, a table analogous to the earlier tables (4.2), (4.3) and (4.5) would be of no use for those z not mentioned, and hence is not reported.

Extreme values of z

As with the t statistic, efficiency problems can arise for extreme values:

- If $z \uparrow 0$ the number of summands needed from the series in j grows to ∞, as is seen from the bound (3.5). Compared with the t statistic, the growth of the truncation order $J(z)$ is slower, but more summands are needed to approximate each $F_j(z)$ because $K_j(z) \geq j$, as mentioned. Still, an efficient and accurate approximation of $F_\kappa(z)$ is possible at least until $z = -0.001$.

- Much as for the t statistic, the approximation finally becomes inefficient as $z \to -\infty$ because, while from the series in j the first summand $F_0(z)$ suffices at high precision, more and more summands $F_{0k}(z)$

[12] To see this, note that (for $K \geq j$ and $y := \sqrt{2|z|}$)

$$\sum_{j=K}^{\infty} F_{jk}(z) = 2\sqrt{\frac{y}{\pi}}\binom{-1/2}{j} e^{-y^2(j^2-j/2-7/16)} \sum_{k=K}^{\infty} y^k D_{-k-3/2}\left(y(2j+3/2)\right),$$

which by our bound (written as in (3.8)) and by using that $j^2 - j/2 - 7/16 = (2j+1/2)^2/2 - (2j+3/2)^2/4$ is in absolute value smaller than

$$2\sqrt{\frac{y}{\pi}}\left|\binom{-1/2}{j}\right| e^{-y^2(2j+1/2)^2/2} \frac{y^K}{\Gamma(K+3/2)} \int_0^{\infty} e^{-ty(2j+1/2)-t^2/2} t^{K+1/2} dt.$$

The latter upper bound is indeed decreasing in j.

are needed to approximate $F_0(z)$. However, even for $z = -40$ we have $|\sum_{k=100}^{\infty} F_{jk}(-40)| < 10^{-6}$, so that the number of summands is still moderate for $z = -40$, which is way beyond all common quantiles. Most importantly, it should be mentioned that the recurrence relation (4.6), if used to compute the parabolic cylinder function, produces sharply increasing relative errors at each step, and a stability test as described in Appendix F should be built in; the author found that, to compensate for the numerical instability, a floating point precision of over 30 digits is required when $z = -15$, and one of at over 60 digits is needed when $z = -40$.

4.4.2 Case of $z > 0$: numerical implementation of Theorem 2.15

For the case $z > 0$ Theorem 2.15 writes $F_\kappa(z)$ as $-1 + \sum_{j=0}^{\infty} F_j(z)$ and gives two expressions of the form $\sum_{k=0}^{\infty} F_{jk}(z)$ for $F_j(z)$. Although we do not possess truncation error bounds, the author has numerically tested the convergence behaviour of the occurring series. Overall, one observes much less efficient convergences than for $z < 0$ or for the formulae for $F_\tau(z)$.

The outer series
As pointed out at the beginning of Section 2.3.4, it clearly seems that $\sum_{j=0}^{\infty} F_j(z)$ also converges when $0 < z \leq 1/2$ (where Theorem 2.15 has not been proven). There is no apparent change in convergence behaviour in the neighbourhood of $z = 1/2$. It moreover seems that the convergence is indeed to the correct value, i.e. that $F_\kappa(z) = -1 + \sum_{j=0}^{\infty} F_j(z)$ holds for *all* $z > 0$.

Whatever the value of $z > 0$, many more than 50 summands in j appear to be necessary to meet even low standards of accuracy. The appropriate truncation order $J = J(z)$ tends to ∞ both for $z \downarrow 0$ and for $z \to \infty$ and seems to reach its minimum far to the left of the 90%-quantile of $z \approx .93$. For z in the region of the commonly required quantiles, already hundreds or even thousands of summands in j are necessary.

The inner series
For the inner series, it is probably advisable to use the second presented series in k of Theorem 2.15; as in the case of $z < 0$ (cf. Section 4.4.1), advantages over the first expression are related to the fact that the finite sum in l is restricted to the coefficient $c(j, k)$ which can be evaluated in a stable way using

(2.32)-(2.33). Hence let $F_j(z) = \sum_{k=0}^{\infty} F_{jk}(z)$ be the second series of Theorem 2.15.

The larger z is, the slower $F_j(z) = \sum_{k=0}^{\infty} F_{jk}(z)$ seems to converge. This convergence rate seems to deteriorate as j increases, unlike for $z < 0$ or for the approximation of $F_\tau(z)$. As a consequence, as j increases, despite $|F_j(z)|$ tends to decrease, surprisingly the truncation order K_j needed to approximate $F_j(z) = \sum_{k=0}^{\infty} F_{jk}(z)$ increases (for large z sharply). Only for very small z does K_j slowly grow in j and is possibly much below j; already when $z > 0.1$ the number K_j is easily larger than j; in the region of the 90%-quantile ($z \approx .93$) K_j usually exceeds $5j$, so that one needs at least $\sum_{j=0}^{J} 5j = 5(J+1)J/2$ summands and hence more than 10^6 summands when $J \geq 650$.

Further, for z below, say, 0.7, a numerical instability can result from the fact that the summands $F_{jk}(z)$, $k \in \mathbf{N}$, may become extremely large in absolute value, although their sum $F_j(z) = \sum_{k=0}^{\infty} F_{jk}(z)$ is small. More precisely, it seems that, as $j \to \infty$, the maximum $\max_{n\in\mathbf{N}} |F_{jk}(z)|$ tends to ∞ although the sum $F_j(z)$ tends to 0. This problem seems not to occur when $z \geq 3/4$ and hence in particular in the region of commonly used quantiles.

Finally, if using the recurrence relation to evaluate the parabolic cylinder function in $F_{jk}(z)$, given the possibly very high number of necessary recursion steps it is particularly important to prevent error explosion (for instance via the techniques of Appendix F).

4.4.3 Case of $z < 0$: numerical implementation of Theorem 2.17

The formula of Theorem 2.17, valid for $z < 0$, involves a single infinite series (in j), say $F_\kappa(z) = \sum_{j=0}^{\infty} F_j(z)$, which should be truncated as discussed in Section 3.2.3. Since $F_j(z)$ contains two finite summations of the form $F_j(z) = \sum_{k=0}^{j} \sum_{l=0}^{k} F_{jkl}(z)$, the total number of summands to be calculated in an approximation $F(z) \approx \sum_{j=0}^{J} F_j(z)$ is of the order $O(J^3)$. For this reason it is fortunate that it turns out that J can be chosen relatively low (except for extreme values of z). This is partly due to the strength of the truncation error bound which prevents a significant overestimation of the truncation order J.

At least when $z \in [-25, -0.005]$, the computation is efficient, J being below 100 even at high precision such as $p = 10^{-10}$. Unlike in the two-series expression (cf. Section 4.4.1), J tends to ∞ not only for $z \uparrow 0$ but also for $z \to -\infty$. The minimum value for J is reached around $z = -0.1$ where J is roughly around 10 at any common precision p. The growth of J as z approaches either 0 or $-\infty$ is relatively slow, and provided that the level of accuracy is not chosen extremely high the computation of $F_\kappa(z)$ is even possible beyond the range $[-25, 0.005]$ with a certain loss of efficiency.

The author is unable to derive the precise intervals on which the error bound is a decreasing respectively increasing function of z. The table below has a different type than the Tables 4.2, 4.3 and 4.5: it contains for certain *intervals* $[a, b] \subset \mathbf{R}_-$ truncation orders J for which numerical tests clearly indicate (but not prove) that when $z \in [a, b]$ then our bound for $\varepsilon(J) := \sum_{j=J+1}^{\infty} F_j(z)$ (and hence $\varepsilon(J)$ itself) is bounded by 10^{-5} respectively 10^{-10}.

	$z \in$ $[-25, -.0005]$	$z \in$ $[-15, -.001]$	$z \in$ $[-7, -.002]$	$z \in$ $[-2, -.006]$
$\lvert\varepsilon\rvert < 10^{-5}$	70	50	35	20
$\lvert\varepsilon\rvert < 10^{-10}$	100	70	50	30

Table 4.6: Truncation orders in the "one series" expression for F_κ

4.4.4 Numerical comparison of the formulae of Theorems 2.11 and 2.17

While the approximation using the one-series expression (Theorems 2.11) and the two-series expression (Theorem 2.17) usually both are very efficient and accurate, efficiency problems can arise when $z \uparrow 0$ or $z \to -\infty$. For $z \uparrow 0$ the number J of needed summands from the series in j both times grows to infinity; the author has found the one-series formula more efficient for z say in $(-0.05, 0)$. As $z \to -\infty$, the approximation finally becomes inefficient too, for the one-series formula because $J \to \infty$ and for the two-series formula because, while J is 0 at even high precision, more and more summands in k are needed to approximate $F_0(z)$. When z is beyond say -25, the one-series formula becomes inefficient. By contrast the two-series formula is still efficient when $z = -40$: for instance, $|\sum_{k=100}^{\infty} F_{jk}(-40)| < 10^{-6}$, i.e. 100 summands suffice at precision 10^{-6}.

Chapter 5

Conclusion

This thesis has investigated Dickey-Fuller distributions in autoregressive models without deterministics. These distributions arise when testing the hypothesis of a unit root in a time series, which is particularly relevant to econometrics.

The analytical forms derived for these distribution functions are integral-free, but involve at least one infinite summation. They also contain a higher transcendental function which is either an incomplete gamma function (for F_τ) or the parabolic cylinder function (for F_κ). Similar forms have been derived by Abadir (1993, 1995). Each expression derived here or by Abadir is valid only for one sign of the argument. This is a consequence of the nature of the expansions performed here and by Abadir and does not mean that Dickey-Fuller distributions have special properties at the origin $z = 0$ (such as some unsmoothness of the distribution function).

Regarding F_τ, the author as well as Abadir were unable to derive closed expressions for positive z. Our formula for negative z involves a Leibniz series, which provides a comfortable truncation criterion.

Regarding F_κ, we derived the first closed expression valid for positive z, as well as the first closed expression valid for negative z and involving a single infinite summation.

Differentiation of expressions for F_τ and F_κ, yields formulae for the densities f_τ and f_κ which contain the same number of infinite summations and tend to be more complicated.

The derived expressions show no apparent analytical structure. It seems difficult and with the techniques presented here perhaps impossible to derive any simple summation-free closed expression in terms of elementary and special functions. The question of whether such expressions exist for Dickey-Fuller distributions is left open.

In those formulae that are valid for negative z, the convergence rates of the series were seen to be sufficiently fast to allow a highly accurate numerical evaluations based on provided truncation error bounds; in the expressions with two series, usually the outer series can be truncated after the first summand. For negative z, inefficiency only occurs when z is extremely close to 0 or so far from 0 that $F_\tau(z)$ respectively $F_\kappa(z)$ becomes extremely small. By contrast, for positive z the expressions for $F_\kappa(z)$ contain very slowly converging series, and the author was unable to derive suitable truncation error bounds.

The limits of the pursued approach can be seen from the various difficulties encountered when $z > 0$: In this case, no expression could be derived for τ, and our expressions for κ are only proven when $z > 1/2$ and have no clear series truncation criteria.

Using our formulae for negative z, we provided tables of quantiles of τ and κ, ranging from the 0.001%-quantile to the 65%-quantile. These tables are more accurate than those in the literature and for the first time contain quantiles far below the 1%-quantile. These very low quantiles can in some cases be used to reject the null hypothesis beyond any reasonable doubt.

Appendix A

Special Functions

- Pochhammer's symbol (Temme, 1996, p. 72):

$$(a)_n := a \cdot (a+1) \cdot \ldots \cdot (a+n-1) = \Gamma(a+n)/\Gamma(a), \quad a \in \mathbf{C}, n \in \mathbf{N}.$$

- The Hermite polynomial (Gradshteyn and Ryzhik, 1994, p. 1057, 8.950):

$$H_n(\zeta) := (-)^n e^{\zeta^2} \frac{d^n}{d\zeta^n} \left\{ e^{-\zeta^2} \right\}, \quad \zeta \in \mathbf{C}, n \in \mathbf{N}.$$

- The incomplete gamma functions (Gradshteyn and Ryzhik, 1994, p. 949, 8.350):

$$\gamma(p,\zeta) := \int_0^\zeta t^{p-1} e^{-t} dt, \quad \zeta \in \mathbf{C}, \operatorname{Re} p > 0,$$
$$\Gamma(p,\zeta) := \int_\zeta^\infty t^{p-1} e^{-t} dt, \quad \zeta, p \in \mathbf{C}.$$

The function $\Gamma(p,\zeta)$ is used to express $F_\tau(z)$. It satisfies the functional relations $\Gamma(p+1,\zeta) - p\Gamma(p,\zeta) - \zeta^p e^{-\zeta} = 0$ and $\frac{d}{d\zeta}\Gamma(p,\zeta) = -\zeta^{p-1} e^{-\zeta}$

- The error function (Gradshteyn and Ryzhik, 1994, p. 938, 8.250):

$$\operatorname{erf}(\zeta) := \frac{2}{\sqrt{\pi}} \int_0^\zeta e^{-t^2} dt = \frac{1}{\sqrt{\pi}} \gamma(1/2, \zeta^2), \quad \zeta \in \mathbf{C}.$$

- The hypergeometric series (Gradshteyn and Ryzhik, 1994, p. 1071):

$$ {}_kF_m(a_1,...,a_k;b_1,...,b_m;\zeta) := \sum_{n=0}^{\infty} \frac{(a_1)_n \cdots (a_k)_n}{n!(b_1)_n \cdots (b_m)_n}\zeta^n, $$

  where $\zeta, a_1, ..., a_k \in \mathbf{C}$ and $b_1, ..., b_m \in \mathbf{C} \setminus \{0, -1, -2, ...\}$ and $m, k \in \mathbf{N}$. This series has convergence radius ∞ if $k \leq m$, convergence radius 1 when $k = m+1$, and convergence radius 0 if $k > m+1$.

- The parabolic cylinder function (Gradshteyn and Ryzhik, 1994, p. 1092-95, or Erdélyi. 1953, vol. 2, p. 117):

$$ \begin{aligned} D_p(\zeta) :=& 2^{\frac{p}{2}} e^{-\frac{\zeta^2}{4}} \left\{ \frac{\sqrt{\pi}}{\Gamma(1/2-p/2)}\, {}_1F_1\left(-\frac{p}{2}, \frac{1}{2}; \frac{\zeta^2}{2}\right) \right. \\ & \left. - \frac{\sqrt{2\pi}\zeta}{\Gamma(-p/2)}\, {}_1F_1\left(\frac{1-p}{2}, \frac{3}{2}, \frac{\zeta^2}{2}\right) \right\}, \quad \zeta, p \in \mathbf{C}. \end{aligned} $$

  This function is used to express $F_\kappa(z)$. It satisfies the functional relations $D_{p+1}(\zeta) - \zeta D_p(\zeta) + pD_{p-1}(\zeta) = 0$ and $D_p'(\zeta) + \zeta D_p(\zeta)/2 - pD_{p-1}(\zeta) = 0$, as well as the differential equation $u''(\zeta) + (p + 1/2 - \zeta^2/4)u(\zeta) = 0$. It generalises Hermite polynomials in the sense that

$$ D_n(\zeta) = -2^{-n/2} e^{-\zeta^2/4} H_n\left(\frac{\zeta}{\sqrt{2}}\right), \quad n \in \mathbf{N},\ \zeta \in \mathbf{C}. $$

- Abadir (1993) introduces the related function

$$ K(p,\zeta) := e^{\zeta^2/4} D_p(\zeta), \quad \zeta, p \in \mathbf{C}. $$

- The modified Bessel function $K_p(\zeta)$ can when $\mathrm{Re}(\zeta) > 0$ be defined by the integral (Gradshteyn and Ryzhik, 1994, p. 968, 8.432):

$$ K_p(\zeta) := \int_0^\infty e^{-\zeta \cosh(t)} \cosh(pt)dt, \quad p \in \mathbf{C},\ \mathrm{Re}\,\zeta > 0. $$

Appendix B

Fourier and Laplace Transforms

Here we define Laplace and Fourier transforms of functions and Borel measures. The literature is not consistent on whether to use a "+" or a "−" in the exponent. At least in Functional Analysis, the more common convention (which we adopt) is a "−". However, mostly a "+" is used to define characteristic functions or moment generating functions of random variables or vectors. Since we always use a "−", to avoid confusion we do not talk of "characteristic functions" or "moment generating functions" of random variables or vectors, but of their Fourier transforms respectively Laplace transforms.

Laplace transforms.

Our notion of a Laplace transform is, in general, bilateral[1].

- Given a bounded (positive or signed or complex) Borel measure μ on the Borel sets of $\mathbf{R}^n$ (e.g. a probability measure), if for a $p \in \mathbf{C}^n$ the (Lebesgue-)integral

$$\bar{\mu}(p) := \int_{\mathbf{R}^n} \exp(-p'x)d\mu(x)$$

exists, then it defines the Laplace transform of μ in p.

- Given a (real- or complex-valued) measurable function f on $\mathbf{R}^n$ (e.g. a probability density function), the Laplace transform of f is defined as the Laplace transform of the Borel measure μ with density f. More precisely,

[1]For instance, in the 1-dimensional case a Laplace transform always is an integral over some interval (a, ∞), and the transform is bilateral if $a = -\infty$ and unilateral if $a = 0$.

if for a $p \in \mathbf{C}^n$ the (Lebesgue-)integral

$$\bar{f}(p) := \int_{\mathbf{R}^n} \exp(-p'x) f(x) dx$$

exists, then it defines the Laplace transform of f in p.

- Given a random vector $X = (X_1, ..., X_n)$ in $\mathbf{R}^n$, its (joint) Laplace transform is defined as the Laplace transform $\bar{P}_X$ of its probability distribution P_X. More precisely, if for a $p \in \mathbf{C}^n$ the (Lebesgue-)integral

$$E\{\exp(-pX)\} = \int_{\mathbf{R}^n} \exp(-p'x) dP_X(x) = \bar{P}_X(p)$$

exists, then it defines the (joint) Laplace transform of X.

Fourier transforms

Note that the defined Laplace transforms $\bar{\mu}(p)$, $\bar{f}(p)$ and $E\{\exp(-pX)\}$ exist when $p \in (i\mathbf{R})^m$, provided that $f \in \mathcal{L}^1(\mathbf{R}^n)$ (e.g. a density function). The functions from $\mathbf{R}^n$ to $\mathbf{C}$ defined by

$$\hat{\mu}(a) := \bar{\mu}(ia), \quad \hat{f}(a) := \bar{\mu}(ia), \quad E\{\exp(-ia)\}$$

are, respectively, the *Fourier transformations*[2] of μ, f and X.

Apart from the different sign in the exponent, the Laplace respectively Fourier transform of X corresponds to the moment generating respectively characteristic function of X.

An inversion formula

Lemma B.1 *Let $b, B > 0, A \in \mathbf{C}$ and $\nu \in \mathbf{R}$. Then*

$$\frac{1}{2\pi i} \int_{b-i\infty}^{b+i\infty} \exp\left[B^2 p^2\right] \exp\left[Ap\right] p^\nu \, dp = \frac{B^{-\nu-1}}{2^{\frac{\nu}{2}+1}\sqrt{\pi}} \exp\left[\frac{-A^2}{8B^2}\right] D_\nu\left(\frac{-A}{\sqrt{2}B}\right).$$

If in particular $\nu = k \in \{0, 1, ...\}$, then

$$\frac{1}{2\pi i} \int_{b-i\infty}^{b+i\infty} \exp\left[B^2 p^2\right] \exp\left[Ap\right] p^k \, dp = \frac{(-1)^k B^{-k-1}}{2^{k+1}\sqrt{\pi}} \exp\left[\frac{-A^2}{4B^2}\right] H_k\left(\frac{A}{2B}\right).$$

[2] The transformation $\mu \mapsto \hat{\mu}$ defines a one-to-one linear function from the bounded Borel measures on $\mathbf{R}^n$ into the *bounded* and *uniformly continuous* function on $\mathbf{R}^n$; moreover, $\hat{f}$ vanishes at infinity for all $f \in \mathcal{L}^1(\mathbf{R}^n)$ (Petersen, 1983, p. 67 & 74).

See Appendix A for the parabolic cylinder function $D_p(\zeta)$.

PROOF: Suppose first that A is real and negative. Then in

$$K = \frac{1}{2\pi i} \int_{b-i\infty}^{b+i\infty} \exp\left[B^2 p^2\right] \exp\left[Ap\right] p^\nu \, dp$$

we can by a triangle argument replace the path by a new path, γ, which corresponds to the square root of the old path. Then substituting $\sqrt{q}$ for p, the path is retransformed into the old path, and

$$K = \frac{1}{2} \left\{ \frac{1}{2\pi i} \int_{b-i\infty}^{b+i\infty} \exp\left[B^2 q\right] \exp\left[A\sqrt{q}\right] q^{\frac{\nu-1}{2}} \, dq \right\} .$$

The claimed relation now follows from Prudnikov and Brychkov and Marichev (1992), p. 52, 10.

This relation, which so far is proven for $A < 0$, holds for all $A \in \mathbf{C}$ because both sides are entire (i.e. on $\mathbf{C}$ holomorphic) functions ($D_\nu(.)$ is entire by Erdélyi (1953, vol. 2, p. 117).

The case where $\nu = k$ is a nonnegative integer is analogous and uses Prudnikov and Brychkov and Marichev (1992), p. 52, 10. **QED**.

Appendix C

Complement to Section 1.3.6

We here give a concise summary of the model generalisations (mentioned in Section 1.4) which lead to the same asymptotic distributions of unit root tests.

Augmented Dickey-Fuller tests
Dickey and Fuller (1979, 1981) propose to control for serial correlation by (for some $p \geq 1$) considering the $AR(p)$ process $X_t, t = 0, ..., T$ satisfying:

$$X_t = \phi_1 X_{t-1} + ... + \phi_p X_{t-p} + \eta_t, \quad t = q, ..., T, \tag{C.1}$$

where η_t is an independent identically distributed sequence with mean 0 and finite fourth moment. This equation can be transformed into:

$$X_t = \alpha X_{t-1} + \zeta^1 \Delta X_{t-1} + ... + \zeta^{p-1} \Delta X_{t-p+1} + \eta_t, \tag{C.2}$$

where $\alpha := \phi_1 + ... + \phi_p$ and $\zeta^j := -(\phi_{j+1} + ... + \phi_p)$ for $j = 0, ..., p-1$. The linear reparameterisation (C.2) has the advantage that the unit root hypothesis simply has the form $\alpha = 1$: indeed, the "lag polynomial" in (C.1), viz. $1 - \phi_1 z - ... - \phi_p z^p$, is 0 in $z = 1$ if and only if $\alpha = 1$. To test the unit root hypothesis $H_0 : \alpha = 1$, Dickey and Fuller's advice is to estimate the model (C.2) by standard OLS, and based on the estimates $\hat{\alpha}_T$, $\hat{\zeta}_T^1, ..., \hat{\zeta}_T^{p-1}, \hat{\sigma}^2$ to still define the t statistic by $\tau_T := (\hat{\alpha}_T - 1)/\hat{\sigma}_{\hat{\alpha}_T}$, while correcting the definition of κ_T as follows:

$$\kappa_T := \frac{T(\hat{\alpha}_T - 1)}{1 - \hat{\zeta}_T^1 - ... - \hat{\zeta}_T^{p-1}}.$$

In τ_T, $\hat{\sigma}^2_{\hat{\alpha}_T}$ is the usual OLS estimator for the regression variance $\sigma^2_{\hat{\alpha}_T}$, namely $\hat{\sigma}_T^2$ times the top left element of the $p \times p$ matrix $\left(\sum_t \mathbf{X}_t \mathbf{X}_t'\right)^{-1}$, where $\hat{\sigma}_T^2$

is the OLS estimator of σ^2 and $\mathbf{X}_t$ is the vector of time t regressors, $\mathbf{X}_t := (X_{t-1}, \Delta X_{t-1}, ..., \Delta X_{t-p+1})'$. Under the assumption that the lag polynomial $1 - \phi_1 z - ... - \phi_p z^p$ has one unit root (i.e. that $a = 1$), and that all other roots are stationary, i.e. outside the unit circle, the test statistics τ_T and κ_T have the same limiting distributions as the limiting distributions arising in the AR(1) model of Section 1.2, cf. (1.4).

Phillips-Perron tests

While the Dickey-Fuller approach still assumes the specification of the autoregression order p, Phillips (1987) proposes a very general non-parametric approach. While keeping the AR(1) equation

$$X_t = \alpha X_{t-1} + \eta_t, \quad t = 1, 2, ...,$$

he assumes that the error process $(\eta_t)_{t=1,2,...}$ is subject to the following very general assumptions[1]: (a) $E(\eta_t) = 0$ for all t; (b) $\lambda^2 := \lim_{T\to\infty} T^{-1} E[(\eta_1 + ... + \eta_T)^2]$ exists and is positive; (c) (η_t) is strongly mixing[2] with mixing coefficients α_m, and there exists a $\beta > 2$ satisfying $\sup_t E(|\eta_t|^\beta) < \infty$ and $\sum \alpha_m^{2-2/\beta} < \infty$.

These conditions allow for a wide range of serially dependent as well as heterogeneous[3] errors. The conditions $\sup_t E(|\eta_t|^\beta) < \infty$ and $\sum \alpha_m^{2-2/\beta} < \infty$ control the extent of the heterogeneity respectively of the temporal dependence of the η_t. Note also that, if (η_t) was a white noise process, then λ^2 would simply be the variance of η_t. Those allowed error processes that are stationary (i.e. have constant first and second moments) contain in particular all stationary Gaussian $ARMA(p,q)$ processes (with $p, q < \infty$); another allowed stationary class is all $MA(\infty)$ processes $\eta_t := \sum_{j=0}^\infty \psi_j \tilde{\eta}_{t-j}$, where $\sum_{j=0}^\infty j\,|\psi_j| < \infty$ and the $\tilde{\eta}_j$ are independent and identically distributed with mean 0 and finite fourth moment (Hamilton (1994), p. 505, Proposition 17.3).

Under these model assumptions, Phillips (1987, p. 287) proposes to define the test statistics τ_T and κ_T as:

$$\begin{aligned} \tau_T :=& \frac{\hat{\alpha}_T - 1}{\hat{\lambda}_T \left(\sum_t X_{t-1}^2\right)^{-1/2}} - \frac{\hat{\lambda}_T^2 - \hat{\sigma}_T^2}{2\hat{\lambda}_T \sqrt{T^{-2}\sum_t X_{t-1}^2}}, \\ \kappa_T :=& T(\hat{\alpha}_T - 1) - \frac{\hat{\lambda}_T^2 - \hat{\sigma}_T^2}{2T^{-2}\sum_t X_{t-1}^2}, \end{aligned}$$

[1]These are the conditions in Phillips (1987), Theorem 4.2; we use a different notation, and the symbol σ^2 is used differently.

[2]See H. White (1984) for the definition of strongly mixing.

[3]"heterogeneous" means that the distribution of η_t may depend on t.

where $\hat{\alpha}_T$ is the usual OLS estimator $\left(\sum_t X_{t-1}X_t\right) / \left(\sum_t X_{t-1}^2\right)$ for α, and $\hat{\sigma}_T^2$ is (for instance) the estimator $T^{-1}\sum_t \left(X_t - \hat{\alpha}_T X_{t-1}\right)^2$ for the *average error variance* $\sigma^2 := \lim_{T\to\infty} T^{-1}\sum_{t=1}^T E(\eta_t^2)$, and $\hat{\lambda}_T^2$ is some consistent estimator of λ^2. Phillips (1987) shows the consistency (under $\alpha = 1$) of $\hat{\alpha}_T$ and $\hat{\sigma}_T^2$ and proposes ways to define the consistent estimator $\hat{\lambda}_T^2$ of λ^2. Comparing these definitions of τ_T and κ_T with those definitions in the simple AR(1) model of Section 1.2 with independent $N(0, \sigma^2)$ errors, it is seen that that the first summand of the new κ_T is identical with the old κ_T, while for τ_T the connection is slightly more remote. By Theorem 5.1 in Phillips (1987), the statistics τ_T and κ_T thus redefined have precisely the same Dickey-Fuller limiting distributions obtained for the simple AR(1) model, cf. (1.4).

The power of Phillip's approach is that it can detect unit roots in most general time series. However, note that this model is not a regression model in the usual sense because the regressor X_{t-1} is not independent of the error η_t. Standard OLS estimation of α, which is consistent for $\alpha = 1$, fails to be consistent in the stationary case $|\alpha| < 1$. Since the model is non-parametric with respect to η_t, it cannot fully capture the dynamics of the data generating process; nor can $\hat{\alpha}_T X_T$ be used as a predictor for X_{T+1}.

Appendix D

Proof for Lemma 2.18

This appendix relates to Abadir's (1995) derivation for the distribution of τ. Abadir's starting expression (which we justified in Section 2.4.2) is

$$f_{R,S}(r,s) = \frac{1}{2\pi i}\int_{1+i\mathbf{R}} e^{sv}\left\{\lim_{K\to\infty}\frac{1}{2\pi i}\right.$$

$$\text{(D.1)}\qquad \left.\times\int_{g_v-iK}^{g_v+iK} e^{(r+1/2)u}\left(\cosh\sqrt{2v}+\frac{u}{\sqrt{2v}}\sinh\sqrt{2v}\right)^{-1/2} du\right\} dv.$$

After performing the below discussed series expansion on the integrand, and by assuming interchangeability of summation with both integrations, Abadir finds the expression of Lemma 2.18 by an elementary technical derivation (Abadir, 1995, p. 778-779). As we mentioned after Lemma 2.18, the (only) theoretical difficulty is to prove the interchangeability of the principal-value integral in (D.1) with summation. A proof is given in Proposition D.1 below.

Abadir writes:

$$\begin{aligned}\cosh\sqrt{2v}+\frac{u}{\sqrt{2v}}\sinh\sqrt{2v} &= \frac{e^{\sqrt{2v}}}{2\sqrt{2v}}\left\{\sqrt{2v}\left(1+e^{-2\sqrt{2v}}\right)+u\left(1-e^{-2\sqrt{2v}}\right)\right\}\\ &= \frac{e^{\sqrt{2v}}\left(\sqrt{2v}+u\right)}{2\sqrt{2v}}\left(1+e^{-\sqrt{8v}}\frac{\sqrt{2v}-u}{\sqrt{2v}+u}\right).\end{aligned}$$

Since $\left|e^{-\sqrt{8v}}\right| = e^{-\operatorname{Re}\sqrt{8v}} < 1$ and $\frac{\sqrt{2v}-u}{\sqrt{2v}+u} \to 1$ as $|u|\to\infty$, a sufficiently large $g_v > 0$ ensures that for all $\operatorname{Re} u = g_v$

$$\text{(D.2)}\qquad \sup_{u\in(g_v-i\infty,g_v+i\infty)}\left|e^{-\sqrt{8v}}\frac{\sqrt{2v}-u}{\sqrt{2v}+u}\right| < 1.$$

Hence in (2.43) Abadir can binomially expand:

$$\left(\cosh\sqrt{2v}+\frac{u}{\sqrt{2v}}\sinh\sqrt{2v}\right)^{-1/2}=\sqrt{2}(2v)^{1/4}e^{-\sqrt{2v}/2}\sum_{j=0}^{\infty}s_j(u) \tag{D.3}$$

where
(D.4)

$$s_j(u):=\binom{-1/2}{j}e^{-j\sqrt{8v}}\frac{\left(\sqrt{2v}-u\right)^j}{\left(\sqrt{2v}+u\right)^{j+1/2}}=\binom{j-1/2}{j}e^{-j\sqrt{8v}}\frac{\left(u-\sqrt{2v}\right)^j}{\left(u+\sqrt{2v}\right)^{j+1/2}}.$$

Proposition D.1 *Let* $\operatorname{Re} v>0$ *and* $\tilde{r}:=r+1/2>0$. *Then*
(D.5)

$$\lim_{K\to\infty}\frac{1}{2\pi i}\int_{g_v-iK}^{g_v+iK}\left\{e^{\tilde{r}u}\sum_{j=0}^{\infty}s_j(u)\right\}du=\sum_{j=0}^{\infty}\left\{\lim_{K\to\infty}\frac{1}{2\pi i}\int_{g_v-iK}^{g_v+iK}e^{\tilde{r}u}s_j(u)du\right\}.$$

It will not be possible to prove this Proposition using the dominated convergence theorem: An integrable dominating function cannot exist because by (D.3)

$$e^{\tilde{r}u}\sum_{j=0}^{\infty}s_j(u)=O(|u|^{-1/2})\quad\text{as } |u|\to\infty,\ u\in\mathbf{C},$$

and hence $e^{\tilde{r}u}\sum_{j=0}^{\infty}s_j(u)$ is not Lebesgue-integrable over $(g_v-i\infty,g_v+i\infty)$.

PROOF. First assume that the relation resulting from replacing each $e^{\tilde{r}u}$ by $e^{\tilde{r}g_v}\cos[\operatorname{Im}(\tilde{r}u)]$ in (D.5) holds, and that the relation resulting from replacing each $e^{\tilde{r}u}$ by $e^{\tilde{r}g_v}\sin[\operatorname{Im}(\tilde{r}u)]$ also holds. Then, since $e^{\tilde{r}u}=e^{\tilde{r}g_v}\{\cos[\operatorname{Im}(\tilde{r}u)]+i\sin[\operatorname{Im}(\tilde{r}u)]\}$, the original relation also holds.

We now prove the relation resulting from replacing $e^{\tilde{r}u}$ by $e^{\tilde{r}g_v}\cos[\operatorname{Im}(\tilde{r}u)]$, namely

$$\begin{aligned}&\lim_{K\to\infty}\frac{1}{2\pi i}\int_{g_v-iK}^{g_v+iK}\left\{e^{\tilde{r}g_v}\cos[\operatorname{Im}(\tilde{r}u)]\sum_{j=0}^{\infty}s_j(u)\right\}du\\ &=\sum_{j=0}^{\infty}\left\{\lim_{K\to\infty}\frac{1}{2\pi i}\int_{g_v-iK}^{g_v+iK}e^{\tilde{r}g_v}\cos[\operatorname{Im}(\tilde{r}u)]s_j(u)du\right\}.\end{aligned} \tag{D.6}$$

The analogous relation involving sin instead of cos can be proven similarly.

The proof consists of the following steps:

- Step A: We assume v is real and positive and write the j^{th} summand on the right hand side of (D.6) as a positive multiple of a series, viz. as $k\sum_{m=0}^{\infty} a_m$.
- Step B: For each j we determine an m_j such that $\sum_{m=0}^{\infty} a_m$ is a Leibniz series up from m_j (i. e. from $m \geq m_j$ the signs of the a_m's are alternating and $|a_m| \downarrow 0$).
- Step C: Still for $v > 0$, we deduce (D.6).
- Step D: We generalise (D.6) to $\operatorname{Re} v > 0$.

Step A
We first prove this Lemma.

Lemma D.2 *For all $K > 0$,*

$$\begin{aligned} &\frac{e^{\tilde{r}g_v}}{2\pi i}\int_{g_v-iK}^{g_v+iK}\left\{\cos[\operatorname{Im}(\tilde{r}u)]\sum_{j=0}^{\infty} s_j(u)\right\}du \\ &= \sum_{j=0}^{\infty}\left\{\frac{e^{\tilde{r}g_v}}{2\pi i}\int_{g_v-iK}^{g_v+iK}\cos[\operatorname{Im}(\tilde{r}u)]s_j(u)du\right\}. \end{aligned} \tag{D.7}$$

Proof. The series $\sum_{j=0}^{\infty} s_j(u)$ equals $\left(\sqrt{2v}+u\right)^{-1/2}$ times a power series in $z(u) := e^{-4\sqrt{v}}(\sqrt{2v}-u)/(\sqrt{2v}+u)$, where by $\operatorname{Re} u = g_v$ and (D.2) $z(u)$ belongs to some compact subset of the disc of convergence of this power series (with radius 1). So this power series and hence also $\sum_{j=0}^{\infty}\cos[\operatorname{Im}(\tilde{r}u)]s_j(u)$ converge uniformly in u where $\operatorname{Re} u = g_v$. This implies (D.7). **QED**.

Now suppose $v > 0$. By substituting $u = g_v + i\pi w/\tilde{r}$ in (D.7) and applying limits on both sides,

$$\begin{aligned} &\lim_{L\to\infty}\frac{e^{\tilde{r}g_v}}{2\tilde{r}}\int_{L}^{L}\left\{\cos(\pi w)\sum_{j=0}^{\infty} s_j(g_v+i\pi w/\tilde{r})\right\}dw \\ &= \lim_{L\to\infty}\sum_{j=0}^{\infty}\left\{\frac{e^{\tilde{r}g_v}}{22\tilde{r}}\int_{-L}^{L}\cos(\pi w)s_j(g_v+i\pi w/\tilde{r})dw\right\}, \end{aligned}$$

and we finally need to show that, on the right hand side, the limit in L can be applied termwise. In other word, by restricting L to a lattice, we have to prove that

$$\lim_{n\to\infty} I_n \text{ exists and } \lim_{n\to\infty}\sum_{j=0}^{\infty} I_n = \sum_{j=0}^{\infty}\lim_{n\to\infty} I_n, \tag{D.8}$$

where for all $n \in \mathbf{N}$

$$I_n := I_n(j,v) := \frac{e^{\tilde{r}g_v}}{2\tilde{r}}\int_{-1/2-n}^{1/2+n}\cos(\pi w)s_j(g_v + i\pi w/\tilde{r})dw$$

This will be achieved through writing $\lim_{n\to\infty} I_n$ as a series $k\sum_{m=0}^{\infty} a_m$ (this step), which will be shown to have the Leibniz property (step B). For all $n \in \mathbf{N}$ write

$$\begin{aligned} I_n &= \frac{e^{\tilde{r}g_v}}{2\tilde{r}}\int_0^{1/2+n}\cos(\pi w)\left\{s_j(g_v + i\pi w/\tilde{r}) + e^{-i\pi w}s_j(g_v - i\pi w/\tilde{r})\right\}dw \\ &= \frac{e^{\tilde{r}g_v}}{\tilde{r}}\int_0^{1/2+n}\cos(\pi w)\,\mathrm{Re}\left\{s_j(g_v + i\pi w/\tilde{r})\right\}dw, \end{aligned}$$

where we used that $s_j(\bar{u}) = \overline{s_j(u)}$ when $v > 0$. Hence

$$I_n = \frac{e^{\tilde{r}g_v}}{\tilde{r}}\left[a_0 + a_1 + ... + a_n\right]$$

with

$$\begin{aligned} a_0 &:= \int_0^{1/2}\cos(\pi w)\,\mathrm{Re}\left\{s_j(g_v + i\pi w/\tilde{r})\right\}\,dw, \\ a_m &:= \int_{m-1/2}^{m+1/2}\cos(\pi w)\,\mathrm{Re}\left\{s_j(g_v + i\pi w/\tilde{r})\right\}\,dw, \quad m \geq 1. \end{aligned}$$

Since $\cos(\pi w)$ has constant sign on $(m-1/2, m+1/2)$, the mean value theorem for integrals can be applied, according to which there exists a $\phi_m \in [m-1/2, m+1/2]$ such that for $m \geq 1$

$$\begin{aligned} a_m &= \mathrm{Re}\left\{s_j(g_v + i\pi\phi_m/\tilde{r})\right\}\int_{m-1/2}^{m+1/2}\cos(\pi w)\,dw \\ &= (-)^m\frac{2}{\pi}\,\mathrm{Re}\left\{s_j(g_v + i\pi\phi_m/\tilde{r})\right\}. \end{aligned}$$

Since g_v was chosen arbitrarily satisfying (D.2), we can here choose g_v to be any positive real (this is because $\sqrt{2v} > 0$ by $v > 0$). Let $g_v := \sqrt{2v}$. Also letting $a := \pi/\tilde{r}$ and $b := 2\sqrt{2v}$, by (D.4) we obtain

$$s_j(g_v + i\pi\phi_m/\tilde{r}) = s_j(b/2 + ia\phi_m) = \binom{j-1/2}{j} e^{-j\sqrt{8v}} \frac{(ia\phi_m)^j}{(ia\phi_m + b)^{j+1/2}},$$

and hence

$$a_m = (-)^m \frac{2}{\pi} \binom{j-1/2}{j} e^{-j\sqrt{8v}} \operatorname{Re}\left\{ \frac{(ia\phi_m)^j}{(ia\phi_m + b)^{j+1/2}} \right\}. \tag{D.9}$$

Step B

Now we determine an $m_j \in \mathbf{N}$ from where the a_m's have the Leibniz property, more precisely from where the real part in a_m is decreasing (its convergence towards 0 being clear from $\phi_m \to \infty$). Write

$$\frac{(ia\phi_m)^j}{(ia\phi_m + b)^{j+1/2}} = g(\phi_m^{-1}),$$

where

$$g(\lambda) := i^{-1/2} a^{-1/2} \lambda^{1/2} \left(1 - iba^{-1}\lambda\right)^{-j-1/2} \quad \forall \lambda > 0.$$

We have to find a right neighbourhood of 0 in which $\operatorname{Re} g(\lambda)$ is increasing. This function (although nowhere holomorphic if λ was allowed to become complex) is $\mathbf{R}$-differentiable: by the continuity and $\mathbf{R}$-linearity of Re on $\mathbf{C}$,

$$\begin{aligned}
\frac{d}{d\lambda} \operatorname{Re} g(\lambda) &= \operatorname{Re} \frac{d}{d\lambda} g(\lambda) \\
&= \operatorname{Re}\left[i^{-1/2} a^{-1/2} \left\{ \frac{1}{2} \lambda^{-1/2} \left(1 - iba^{-1}\lambda\right)^{-j-1/2} \right.\right. \\
&\qquad \left.\left. + \lambda^{1/2} iba^{-1} \left(j + \frac{1}{2}\right) \left(1 - iba^{-1}\lambda\right)^{-j-\frac{3}{2}} \right\}\right] \\
&= \frac{1}{2} a^{-1/2} \lambda^{-1/2} \operatorname{Re}\left[i^{-1/2} \left(1 - iba^{-1}\lambda\right)^{-j-1/2} \right. \\
&\qquad \left. \times \left\{ 1 + 2\left(j + \frac{1}{2}\right) \frac{iba^{-1}\lambda}{1 - iba^{-1}\lambda} \right\} \right].
\end{aligned} \tag{D.10}$$

Lemma D.3 *$\frac{d}{d\lambda}\operatorname{Re} g(\lambda) \geq 0$ for*

$$0 < \lambda \leq B(j) := (2j+1)^{-1} b^{-1} a. \tag{D.11}$$

Proof. Let $\lambda > 0$. By (D.10), $\frac{d}{d\lambda}\operatorname{Re} g(\lambda) \geq 0$ if and only if

$$\theta := \arg\left[i^{-1/2}\left(1 - iba^{-1}\lambda\right)^{-j-\frac{1}{2}}\left\{1 + 2\left(j + 1/2\right)\frac{iba^{-1}\lambda}{1 - iba^{-1}\lambda}\right\}\right] \in \left[-\frac{\pi}{2}, \frac{\pi}{2}\right].$$

We have

$$\theta = -\frac{\pi}{4} + \frac{1}{2}\left(2j+1\right)\arg z_1 + \arg z_2 \mod 2\pi, \tag{D.12}$$

where

$$\begin{aligned} z_1 :=& 1 + iba^{-1}\lambda, \\ z_2 :=& 1 + (2j+1)\frac{iba^{-1}\lambda - b^2a^{-2}\lambda^2}{1 + b^2a^{-2}\lambda^2} = 1 + 2\left(j + \frac{1}{2}\right)\frac{iba^{-1}\lambda(1 + iba^{-1}\lambda)}{1 + b^2a^{-2}\lambda^2}. \end{aligned}$$

Now assume λ satisfies (D.11). We will deduce bounds for both $\arg z_1$ and $\arg z_2$, and these bounds will imply $\theta \in [-\pi/2, \pi/2]$. Consider first $\arg z_1$. Jordan's inequality says that, if $\psi \in [0, \pi/2]$, then $\psi \leq (\pi/2)\sin\psi$. So, since $\arg z_1 \in [0, \pi/2]$, we have

$$\begin{aligned} \arg z_1 &\leq \frac{\pi}{2}\sin\{\arg z_1\} = \frac{\pi}{2}\frac{ba^{-1}\lambda}{\sqrt{1 + b^2a^{-2}\lambda^2}} \\ &\leq \frac{\pi}{2}ba^{-1}\lambda \leq \frac{\pi}{2}ba^{-1}B(j) = \frac{\pi}{2}\left(2j+1\right)^{-1}. \end{aligned}$$

On the other hand, $\arg z_2 \in [0, \pi/2]$ since $\operatorname{Im} z_2 \geq 0$ and condition (D.11) ensures that

$$\begin{aligned} \operatorname{Re} z_2 &= 1 - (2j+1)\frac{b^2a^{-2}\lambda^2}{1 + b^2a^{-2}\lambda^2} \geq 1 - (2j+1)\, b^2a^{-2}\lambda^2 \\ &\geq 1 - (2j+1)\, b^2a^{-2}B(j)^2 = 1 - (2j+1)^{-1} \geq 0. \end{aligned}$$

Since $\arg z_1 \in [0, (2j+1)^{-1}\pi/2]$ and $\arg z_2 \in [0, \pi/2]$, we deduce from (D.12) that

$$\theta = -\frac{\pi}{4} + \frac{1}{2}\left(2j+1\right)\arg z_1 + \arg z_2 \in \left[-\frac{\pi}{4}, \frac{\pi}{2}\right]. \quad \textbf{QED}.$$

Since $\phi_m \in [m - 1/2, m + 1/2]$, ϕ_m^{-1} is a non-increasing function of m, and so the above Lemma implies that $\operatorname{Re} g(\phi_m^{-1})$ is non-increasing as a function of m provided that $\phi_m^{-1} \leq B(j)$, i.e. provided that $\phi_m \geq B(j)^{-1}$, and hence in particular for

$$m \geq m_j := \lceil B(j)^{-1} + 1/2 \rceil = \lceil (2j+1)\, ba^{-1} + 1/2 \rceil . \tag{D.13}$$

So, by (D.9) (a_m) is Leibniz from $m \geq m_j$. In particular,

$$\lim_{n\to\infty} I_n = \tilde{r}^{-1} e^{\tilde{r} g_v} \sum_{m=0}^{\infty} a_m$$

exists, which is the first part of (D.8).

Step C

To show the second part of (D.8), we write $\lim_{n\to\infty} I_n$ as an absolutely convergent series:

$$\lim_{n\to\infty} I_n = \sum_{m=0}^{\infty} \frac{e^{\tilde{r} g_v}}{\tilde{r}} \left(a_{2m} + a_{2m+1}\right).$$

This series is absolutely convergent because it converges and, by the Leibniz property from $m \geq m_j$, all apart from finitely many summands are of the same sign. The sum of the absolute values is

$$\sum_{m=0}^{\infty} \frac{e^{\tilde{r} g_v}}{\tilde{r}} |a_{2m} + a_{2m+1}| = \frac{e^{\tilde{r} g_v}}{\tilde{r}} \left\{ \sum_{2m < m_j} |a_{2m} + a_{2m+1}| + \sum_{2m \geq m_j} |a_{2m} + a_{2m+1}| \right\},$$

where by the triangle inequality

$$\sum_{2m < m_j} |a_{2m} + a_{2m+1}| \leq \sum_{m \leq m_j} |a_m| , \tag{D.14}$$

and by the Leibniz property

$$\sum_{2m \geq m_j} |a_{2m} + a_{2m+1}| = \left| \sum_{2m \geq m_j} (a_{2m} + a_{2m+1}) \right| = \left| \sum_{m \geq m_j} a_m \right| \leq \left| a_{m_j} \right| . \tag{D.15}$$

Now, from the definition of a_m one easily deduces that

$$|a_m| \leq C \binom{j - 1/2}{j} e^{-j\sqrt{8v}} \leq C e^{-j\sqrt{8v}} \quad \forall m \in \mathbf{N}, \tag{D.16}$$

where $C >$ is a constant that is independent of m, j (but may depend on $v, \tilde{r}$). So

$$\begin{aligned}
\sum_{m=0}^{\infty} \frac{e^{\tilde{r} g_v}}{\tilde{r}} \left| a_{2m} + a_{2m+1} \right| &\leq \frac{e^{\tilde{r} g_v}}{\tilde{r}} \left\{ \sum_{m \leq m_j} |a_m| + \left| a_{m_j} \right| \right\} && \text{by (D.14), (D.15)} \\
&\leq C \frac{e^{\tilde{r} g_v}}{\tilde{r}} (m_j + 2)\, e^{-j\sqrt{8v}} && \text{by (D.16)} \\
&\leq C \frac{e^{\tilde{r} g_v}}{\tilde{r}} \left((2j+1)\, ba^{-1} + \frac{7}{2} \right) e^{-j\sqrt{8v}} && \text{by (D.13).}
\end{aligned}$$

It is obvious that the sum over $j \in \mathbf{N}$ of the last expression is finite. So $\sum_{j=0}^{\infty} \sum_{m=0}^{\infty} \frac{e^{\tilde{r} g_v}}{\tilde{r}} \left| a_{2m} + a_{2m+1} \right|$ is also finite, which implies the convergence of

$$\sum_{j=0}^{\infty} \sum_{m=0}^{\infty} \frac{e^{\tilde{r} g_v}}{\tilde{r}} (a_{2m} + a_{2m+1}) = \sum_{j=0}^{\infty} \lim_{n\to\infty} I_n,$$

as well as the fact that we can reorder the sums to give

$$\sum_{j=0}^{\infty} \lim_{n\to\infty} I_n = \sum_{m=0}^{\infty} \left\{ \sum_{j=0}^{\infty} \frac{e^{\tilde{r} g_v}}{\tilde{r}} (a_{2m} + a_{2m+1}) \right\}.$$

Now, using the inequality (D.16), one can easily see that $\sum_{j=0}^{\infty} \frac{e^{\tilde{r} g_v}}{\tilde{r}} a_{2m}$ converges, which implies that

$$\sum_{j=0}^{\infty} \lim_{n\to\infty} I_n = \sum_{m=0}^{\infty} \left\{ \sum_{j=0}^{\infty} \frac{e^{\tilde{r} g_v}}{\tilde{r}} a_{2m} + \sum_{j=0}^{\infty} \frac{e^{\tilde{r} g_v}}{\tilde{r}} a_{2m+1} \right\} = \sum_{m=0}^{\infty} \sum_{j=0}^{\infty} \frac{e^{\tilde{r} g_v}}{\tilde{r}} a_m.$$

Hence, finally,

$$\begin{aligned}
\sum_{j=0}^{\infty} \lim_{n\to\infty} I_n &= \lim_{n\to\infty} \left\{ \sum_{m=0}^{n} \sum_{j=0}^{\infty} \frac{e^{\tilde{r} g_v}}{\tilde{r}} a_m \right\} \\
&= \lim_{n\to\infty} \left\{ \sum_{j=0}^{\infty} \sum_{m=0}^{n} \frac{e^{\tilde{r} g_v}}{\tilde{r}} a_m \right\} = \lim_{n\to\infty} \sum_{j=0}^{\infty} I_n.
\end{aligned}$$

This completes the proof of (D.8) for real $v > 0$.

Step D

We now have to generalise (D.5) to $\operatorname{Re} v > 0$. This is done by showing that both sides of (D.5) define holomorphic functions of v on $\operatorname{Re} v > 0$. Since these functions coincide on the subset $\mathbf{R}_+$ (which contains limit points), the identity theorem implies that they coincide on the whole of $\operatorname{Re} v > 0$.

The left hand side is holomorphic on $\operatorname{Re} v > 0$ because it is the Laplace inverse, taken in $\tilde{r}$, of a function of the kind $a\,(1+ub)^{-1/2}$, with constants $a := \left[\sqrt{2}(2v)^{1/4}e^{-\sqrt{2v}/2}\right]^{-1}\cosh^{-1/2}\sqrt{2v}$ and $b := \left(\tanh\sqrt{2v}\right)/\sqrt{2v}$; this inverse can be calculated as discussed in Section 2.2, the result being a holomorphic function on $\operatorname{Re} v > 0$.

So far as the right hand side of (D.5) is concerned, the termwise inverses as calculated by Abadir (1995) are holomorphic on $\operatorname{Re} v > 0$; one can easily show that their infinite sum converges locally uniformly in v on $\operatorname{Re} v > 0$ and so the limit is holomorphic on $\operatorname{Re} v > 0$. **QED**.

Appendix E

Proofs for Section 2.4.3

Let $z < 0$. In (2.45) of Section 2.4.3, the limiting density $f_\tau(z)$ is written as a sum of integrals:

$$f_\tau(z) = \frac{1}{\sqrt{\pi}} \sum_{j=0}^{\infty} \binom{j-1/2}{j} \sum_{l=0}^{j} \binom{j}{l} (-2)^l S_{jl}(z)$$

where

$$S_{jl}(z) := \int_{4j+1}^{\infty} \exp\left[-\frac{1}{2} z^2 s^2\right] H_2\left(\frac{zs}{\sqrt{2}}\right) (s+1)^{-l-1/2} ds.$$

From here, Section 2.4.3 proceeds to calculate the distribution function $F_\tau(z) = \int_{-\infty}^{z} f_\tau(z')dz'$ by interchanging the integral in z' first with the infinite sum and then with in integral occurring in $S_{jk}(z)$. In the Lemmata E.1 and E.2 below we proves that both of these interchanges were legitimate.

Lemma E.1 *For all $z < 0$ the distribution function equals*

$$F_\tau(z) = \frac{1}{\sqrt{\pi}} \sum_{j=0}^{\infty} \binom{j-1/2}{j} \sum_{l=0}^{j} \binom{j}{l} (-2)^l \int_{-\infty}^{z} S_{jl}(z')dz'.$$

PROOF. In order to apply the dominated convergence theorem, we first dominate the j^{th} summand of the integrand $f_\tau(z')$: by the binomial formula,

$$\begin{aligned}
&\left|\sum_{l=0}^{j}\binom{j}{l}(-2)^l S_{jl}(z')\right| \\
&= \left|\int_{4j+1}^{\infty}\exp\left[-\frac{1}{2}z'^2s^2\right]H_2\left(\frac{z's}{\sqrt{2}}\right)(s+1)^{-1/2}\left(1-\frac{2}{s+1}\right)^j ds\right| \\
&< \bar{S}_j(z) := 2\int_{4j+1}^{\infty}\exp\left[-\frac{1}{2}z'^2s^2\right]\left(z'^2s^2+1\right)(s+1)^{-1/2}ds,
\end{aligned}$$

where the inequality follows by noting that

$$|H_2(t)| = 2\left|t^2-1\right| \le 2(t^2+1) \quad \text{and} \quad 0 < \frac{2}{s+1} < 1.$$

Our dominating function is

$$\bar{S}(z') := \frac{1}{\sqrt{\pi}}\sum_{j=0}^{\infty}\binom{j-1/2}{j}\bar{S}_j(z').$$

To see that $\bar{S}(z')$ has a finite integral, note first that

$$\begin{aligned}
\int_{-\infty}^{z}\bar{S}(z')dz' &= \frac{1}{\sqrt{\pi}}\sum_{j=0}^{\infty}\binom{j-1/2}{j}\int_{-\infty}^{z}\bar{S}_j(z')dz' \\
&= \frac{2}{\sqrt{\pi}}\sum_{j=0}^{\infty}\binom{j-1/2}{j}\int_{4j+1}^{\infty}\frac{ds}{\sqrt{s+1}} \\
&\qquad\qquad \times \int_{-\infty}^{z}\exp\left[-\frac{1}{2}z'^2s^2\right]\left(z'^2s^2+1\right)dz'.
\end{aligned}$$

Here, the integral in z' was interchanged first with the sum using the monotone convergence theorem, and then with the integral in $\bar{S}_j(z')$ using the fact that the integrand to the double integral is a positive function. The double integral can be bounded as follows:

$$
\begin{aligned}
&\int_{4j+1}^{\infty} \frac{ds}{\sqrt{s+1}} \int_{-\infty}^{z} \exp\left[-\frac{1}{2}z'^2 s^2\right] \left(z'^2 s^2 + 1\right) dz' \\
&= \int_{4j+1}^{\infty} \frac{ds}{s\sqrt{s+1}} \int_{-\infty}^{sz} \exp\left[-\frac{1}{2}z'^2\right] \left(z'^2 + 1\right) dz' \\
&< \left\{\int_{4j+1}^{\infty} \frac{ds}{s^{3/2}}\right\} \left\{\int_{-\infty}^{(4j+1)z} \exp\left[-\frac{1}{2}z'^2\right] \left(z'^2 + 1\right) dz'\right\} \\
&= \frac{2}{\sqrt{4j+1}} \left\{\int_{\frac{1}{2}(4j+1)^2 z^2}^{\infty} \exp\left[-z'\right] (2z'+1) \frac{dz'}{\sqrt{2z'}}\right\} \\
&= \frac{2}{\sqrt{4j+1}} \left\{\sqrt{2}\Gamma\left(\frac{3}{2}, \frac{1}{2}(4j+1)^2 z^2\right) + \frac{1}{\sqrt{2}}\Gamma\left(\frac{1}{2}, \frac{1}{2}(4j+1)^2 z^2\right)\right\}.
\end{aligned}
$$

The last line can be bounded by using the order 0 asymptotic expansion of the incomplete gamma function: By Erdélyi (1953, vol. 2, p. 135, (6)), this expansion is $\Gamma(\alpha, z') = z'^{\alpha-1}e^{-z'}\{1 + o(1)\}$ as $z' \to \infty$; if $\alpha > 0$, then $\Gamma(\alpha, z')$ is a continuous function of $z' \in [\mathbf{0}, \infty[$, and so the expansion implies that there is a constant $k(\alpha) > 0$ such that $\Gamma(\alpha, z') \leq k(\alpha)z'^{\alpha-1}e^{-z'}$ for all $z' \in [0, \infty[$. Applying this, we have

$$
\begin{aligned}
&\int_{4j+1}^{\infty} \frac{ds}{\sqrt{s+1}} \int_{-\infty}^{z} \exp\left[-\frac{1}{2}z'^2 s^2\right] \left(z'^2 s^2 + 1\right) dz' \\
&< \frac{2}{\sqrt{4j+1}} \left\{\sqrt{2}k\left(\frac{3}{2}\right) \left[\frac{1}{2}(4j+1)^2 z^2\right]^{1/2} e^{-\frac{1}{2}(4j+1)^2 z^2}\right. \\
&\qquad \left. + \frac{1}{\sqrt{2}}k\left(\frac{1}{2}\right) \left[\frac{1}{2}(4j+1)^2 z^2\right]^{-1/2} e^{-\frac{1}{2}(4j+1)^2 z^2}\right\} \\
&= 2\left\{|z|k\left(\frac{3}{2}\right)(4j+1)^{1/2} + |z|^{-1}k\left(\frac{1}{2}\right)(4j+1)^{-\frac{3}{2}}\right\} e^{-\frac{1}{2}(4j+1)^2 z^2} \\
&< C_z (4j+1)^{1/2} e^{-\frac{1}{2}(4j+1)^2 z^2},
\end{aligned}
$$

where C_z is a positive constant that depends on z but not on j. The integral of the dominating function now satisfies

$$
I(z) < 2\sum_{j=0}^{\infty} \binom{j-1/2}{j} C_z (4j+1)^{\frac{1}{2}} e^{-\frac{1}{2}(4j+1)^2 z^2} < \infty. \quad \textbf{QED}.
$$

It remains to prove that one may interchange integrals:

Lemma E.2 *For all* $z < 0$, *the order of integration in the double integral* $\int_{-\infty}^{z} S_{jl}(z')dz'$ *can be interchanged.*

PROOF. We have

$$\text{(E.1)} \quad \int_{-\infty}^{z} S_{jl}(z')dz' = \int_{-\infty}^{z} dz' \int_{4j+1}^{\infty} \exp\left[-\frac{1}{2}z'^2 s^2\right] H_2\left(\frac{z's}{\sqrt{2}}\right)(s+1)^{-l-1/2}ds.$$

The integrand of this double integral is in absolute value smaller than the function $2\exp\left[-\frac{1}{2}z'^2s^2\right](z'^2s^2+1)(s+1)^{-1/2}$ which has a finite double integral by the argument in the proof of Lemma E.1. Therefore the integrand in (E.1) is (product-)integrable over $]-\infty, z] \times [4j+1, \infty[$, and the claim follows from the theorem of Fubini. **QED**.

Appendix F

Stability Tests for Recursive Evaluations

Suppose that $F_\kappa(z)$ is for $z < 0$ calculated using the expression of Theorem 2.11. Assume further that the recursion relation

$$D_{p+1}(\zeta) - \zeta D_p(\zeta) + pD_{p-1}(\zeta) = 0 \tag{F.1}$$

is used to calculate the relevant values of the parabolic cylinder function. In this Appendix we explain how rounding errors in this recursion can be controlled. The discussion would be similar for the one series formula for $F_\kappa(z)$, or for the formulae for $F_\kappa(z)$ when $z > 0$, or for the formulae for $F_\tau(z)$ in which the incomplete gamma function can be calculated by recursion (cf. Section 4.2.1).

The danger in the recursion relation (F.1) is not only due to a possible error accumulation after many recursion steps, but also to a possible relative error "explosion" in a single step due to the additive operation. Indeed, given two (non-identical) numbers $a, b \in \mathbf{R}$ for which one has approximations $\hat{a}$ and $\hat{b}$, the relative error of the difference $\hat{b} - \hat{a}$ as an approximation of $b - a$ is

$$\frac{(\hat{b} - \hat{a}) - (b - a)}{b - a} = \frac{(\hat{b} - b) - (\hat{a} - a)}{b - a}$$

which, even if $\hat{b} - b$ and $\hat{a} - a$ are small, may be arbitrarily large if $b - a$ happens to be close 0.

We derive three upper bounds (R_n, R'_n and R''_n) for the relative error contained in the recursively calculated value for $D_p(\zeta)$; only the third of these bounds satisfies all practical needs.

The setting

We write a hat "$\widehat{\ }$" over a quantity or an expression to denote its computer evaluation (usually with errors); the evaluation may consist of many operations following each other: for instance, $\widehat{a+2b} = \widehat{a+\widehat{2b}}$. We define the relative error s of an approximation $\hat{a}$ of a as $s := (\hat{a}-a)/a$, interpreted as 0 if $\hat{a} = a = 0$, as $+\infty$ if $\hat{a} > a = 0$, and as $-\infty$ if $\hat{a} < a = 0$. The identity $\hat{a} = a(1+s)$ holds except when $\hat{a} \neq a = 0$.

In Theorem 2.11, $F_\kappa(z)$ is for $z < 0$ expressed in terms of parabolic cylinder functions of the form

$$D_n := D_{-n-3/2}(\zeta) \quad \text{where } \zeta := \sqrt{2|z|}(2j+3/2) \text{ and } n \in \mathbf{N}.$$

For given $z < 0$ and j, the approximation $\hat{D}_n$ of D_n is calculated as follows: The initial values D_0 and D_1 are calculated directly[1], yielding approximations $\hat{D}_0$ and $\hat{D}_1$, and later values are calculated using the recursion relation

$$D_n = (D_{n-2} - \zeta D_{n-1})/(n+1/2) \quad \forall n \geq 2. \tag{F.2}$$

In other words, the software computes $\hat{D}_n$ by evaluating (with rounding errors) the expression $(\hat{D}_{n-2} - \zeta\hat{D}_{n-1})/(n+1/2)$. An integral representation of the incomplete gamma function (Gradshteyn and Ryzhik, 1994, p. 1092, 9.241) shows that

$$D_n > 0, \quad \forall n \in \mathbf{N}, \tag{F.3}$$

which indicates the possibility of a relative error "explosion" in the difference (F.2). Call r_n the relative error of $\hat{D}_n$, so that $r_n = (\hat{D}_n - D_n)/D_n$ or $\hat{D}_n = D_n(1+r_n)$.

We have to derive a suitable upper bound for $|r_n|$. The idea is that, whenever D_n is updated, the program also updates the bound for $|r_n|$ and checks whether the latter is small enough. If not, then the floating point precision should be increased, resulting in a smaller bound for $|r_n|$ due to smaller values for the parameters R_0, R_1, R and S defined below.

We assume that there are known numbers $R_0, R_1, R, S \in \mathbf{R}$ such that

- $\hat{D}_0$ and $\hat{D}_1$ are correct to relative precisions satisfying $|r_0| \leq R_0$ and $|r_1| \leq R_1$,

[1]See section 4.2.2 for the case that the parabolic cylinder function is not available.

- each elementary operation produces a relative error of at most R in absolute value[2]; in particular, if the correct result is 0, the calculated result is 0;
- the square root in ζ is evaluated to a relative error of at most S in absolute value;
- the terms $n+1/2$, $2j+3/2$ and $2|z|$ (the last two occur in ζ) are evaluated without error.

The last assumption is appropriate given some minimal standards of floating point accuracy together with supposing that n and j do not become extremely large (hence no overflow) and that the input variable z has a reasonably simple form with not too many digits in the mantissa.

The bound R_n for r_n
The following proposition contains a first bound for r_n.

Proposition F.1 *Under the above assumptions, r_n satisfies the inequality $|r_n| \leq R_n$ for all $n \in \mathbf{N}$, where the error bound R_n is given by the recursion formula*

$$R_n := U_n + (1 + U_n)(2R + R^2), \quad \forall n \geq 2,$$

with U_n depending on D_{n-1}, D_{n-2} and R_{n-1}, R_{n-2} via

$$U_n := \frac{D_{n-2}R_{n-2} + \zeta D_{n-1}[R_{n-1} + (1 + R_{n-1})(S + (1 + S)(2R + R^2))]}{D_{n-2} - \zeta D_{n-1}}, \ n \geq 2.$$

Since R is typically very small, R_n is essentially U_n. The possibility of a relative error "explosion" is reflected in the fact that the denominator of U_n can become very small if the two (positive) terms D_{n-2} and ζD_{n-1} may have similar magnitudes.

Proof. We prove by induction that $|r_n| \leq R_n$ for all $n \in \mathbf{N}$. The inequality holds by assumption for $n = 0, 1$. Now let $n \geq 2$. Note first that

$$\text{(F.4)} \qquad \hat{D}_n = \left\{ \left[\hat{D}_{n-2} - \zeta \hat{D}_{n-1}(1 + s) \right] (1 + s')/(n + 1/2) \right\} (1 + s''),$$

where

[2] R could be $0.5 \times 10^{1-d}$, where d is the number of floating point digits used by the software. For istance, if d was only 1, then 1.43 would be rounded to 1, creating a relative error of $(1.43-1)/1.43$, which is indeed less than $0.5 \times 10^{1-d}$.

- s is the relative error from calculating $\zeta = \sqrt{2|z|}(2j+3/2)$ and multiplying the result, $\hat{\zeta}$, with $\hat{D}_{n-1}$,
- s' is the relative error from subtracting $\zeta\hat{D}_{n-1}(1+s)$ from $\hat{D}_{n-2}$,
- s'' is the relative error from dividing $\left[\hat{D}_{n-2} - \zeta\hat{D}_{n-1}(1+s)\right](1+s')$ by $n+1/2$.

Note that by assumption no rounding error occurs in $n+1/2$. In (F.4),

$$\hat{D}_{n-2} - \zeta\hat{D}_{n-1}(1+s) = D_{n-2}(1+r_{n-2}) - \zeta D_{n-1}(1+r_{n-1})(1+s),$$

which can be written as

$$\hat{D}_{n-2} - \zeta\hat{D}_{n-1}(1+s) = (D_{n-2} - \zeta D_{n-1})(1+u_n) \tag{F.5}$$

with

$$u_n := \frac{D_{n-2}r_{n-2} - \zeta D_{n-1}[r_{n-1} + (1+r_{n-1})s]}{D_{n-2} - \zeta D_{n-1}},$$

because $D_{n-2} - \zeta D_{n-1} = (n+1/2)D_n \neq 0$ by (F.3). By substituting (F.5) into (F.4),

$$\hat{D}_n = \left(\frac{D_{n-2} - \zeta D_{n-1}}{n+1/2}\right)(1+u_n)(1+s')(1+s'') = D_n(1+u_n)(1+s')(1+s'').$$

Since $\hat{D}_n$ also equals $D_n(1+r_n)$, we deduce that

$$1 + r_n = (1+u_n)(1+s')(1+s''),$$

or

$$r_n = u_n + (1+u_n)(s' + s'' + s's'').$$

In this we have $|s'| \leq R$ and $|s''| \leq R$. Hence, in order to complete the proof of $|r_n| \leq |R_n|$ it remains to prove that $|u_n| \leq U_n$.

First, we bound s. In calculating $\zeta\hat{D}_{n-1} = \sqrt{2|z|}(2j+3/2)\hat{D}_{n-1}$, by assumption the terms $2j+3/2$ and $2|z|$ are evaluated without error. Hence the only rounding errors occur in the square root (relative error: s_1) and the two outer multiplications (relative errors: s_2, s_3):

$$\zeta\hat{D}_{n-1}(1+s) = \zeta\hat{D}_{n-1}(1+s_1)(1+s_2)(1+s_3).$$

If $\hat{D}_{n-1} \neq 0$, this implies that s can be written as:

$$s = s_1 + (1 + s_1)(s_2 + s_3 + s_2 s_3).$$

By assumption, $|s_1| \leq S$, $|s_2| \leq R$ and $|s_3| \leq R$. Hence

$$|s| \leq S + (1 + S)(2R + R^2). \tag{F.6}$$

If $\hat{D}_{n-1} = 0$, the last inequality holds too since $\zeta \hat{D}_{n-1}$ is evaluated to 0, so that $s = 0$. The inequality $|u_n| \leq U_n$ now follows by using (F.6), the induction hypothesis $|r_{n-1}| \leq R_{n-1}$, $|r_{n-2}| \leq R_{n-2}$, and the fact that by (F.3) all of the terms D_{n-2}, D_{n-1} and $D_{n-2} - \zeta D_{n-1} = (n + 1/2)D_n$ are positive. **QED**.

The bound R'_n for r_n

The bound R_n in Proposition F.1 has two deficiencies, both related to the (recursive) numerical evaluation of R_n:

1. The bound R_n is based on the values D_{n-2} and D_{n-1}, which in the calculation $\hat{R}_n$ are replaced by $\hat{D}_{n-2}$ and $\hat{D}_{n-1}$. If $\hat{D}_{n-2}$ and $\hat{D}_{n-1}$ were much wrong approximations of D_{n-2} and D_{n-1}, so would probably be the approximation $\hat{R}_n$ of R_n.

2. The denominator $D_{n-2} - \zeta D_{n-1}$ appearing in U_n is a difference of positive terms, which contains the danger of numeric instability and hence of a wrong evaluation of R_n.

Both of these potential problems can be avoided by using slightly changed (larger) bounds whose computation can not become lower than the original bound R_n. Let us first tackle the first problem by moving to a bound $R'_n \geq R_n$, and later also tackle the second problem by moving to a bound $R''_n \geq R'_n$.

To prevent the danger mentioned in 1., we define a weaker bound R'_n by replacing each D_i by a suitable new quantity. More precisely, we define R'_n by the following possibly terminating recursion:

(i) For $n = 0, 1$ put $R'_n := R_n$.

(ii) Let $n \geq 2$. If R'_{n-2} and R'_{n-1} are defined and smaller than 1, and in addition

$$E'_n := D_{n-2}/(1 + R'_{n-2}) - \zeta D_{n-1}/(1 - R'_{n-1}) > 0,$$

then R'_n is defined as

$$R'_n := U'_n + (1 + U'_n)(2R + R^2),$$

with U_n' *depending on* D_{n-1}, D_{n-2} *and* R_{n-1}', R_{n-2}' *via*

$$U_n' := \frac{1}{E_n'} \left\{ D_{n-2}R_{n-2}'/(1-R_{n-2}') \right.$$
$$\left. +\zeta D_{n-1}[R_{n-1}' + (1+R_{n-1}')(S+(1+S)(2R+R^2))]/(1-R_{n-1}') \right\}.$$

Otherwise, R_n' *is undefined.*

The fact that the bound R_n' is available only until the recursion terminates is no inconvenience since a recursion termination means that the relative errors may be very large, in which case the calculation of $F_\kappa(z)$ has anyway to be repeated with a higher floating point accuracy. What has changed is that R_i has been replaced either by $D_i/(1+R_i')(\leq D_i)$ or by $D_i/(1-R_i')(\geq D_i)$, depending on whether this D_i has a decreasing or increasing effect on the bound. So, by a straightforward induction, the new bound is weaker:

Corollary F.2 *Under the assumptions of Proposition F.1,* $|r_n| \leq R_n \leq R_n'$ *for all* $n \in \mathbf{N}$ *for which* R_n' *is defined.*

The advantage of R_n' is in the computation: when computation R_n or R_n', each D_i is replaced by $\hat{D}_i = D_i(1+r_i)$, and in R_i' the division by $(1 \pm R_i')$ compensates for the term $(1+r_i)$ since $|r_i| < R_i'$. To formulate this more precisely, let us define the numbers $\tilde{R}_n'$ by exactly the same (possibly terminating) recursion as for R_n', except that now each D_i is replaced by $\hat{D}_i$:

(i) For $n = 0, 1$ *put* $\tilde{R}_n' := R_n$.

(ii) Let $n \geq 2$*. If* $\tilde{R}_{n-2}'$ *and* $\tilde{R}_{n-1}'$ *are defined and smaller than* 1*, and in addition*

$$\tilde{E}_n' := \hat{D}_{n-2}/(1+\tilde{R}_{n-2}') - \zeta\hat{D}_{n-1}/(1-\tilde{R}_{n-1}') > 0,$$

then $\tilde{R}_n'$ *is defined as*

$$\tilde{R}_n' := \tilde{U}_n' + (1+\tilde{U}_n')(2R+R^2),$$

with $\tilde{U}_n'$ *depending on* $\hat{D}_{n-1}$, $\hat{D}_{n-2}$ *and* $\tilde{R}_{n-1}'$, $\tilde{R}_{n-2}'$ *via*

$$\tilde{U}_n' := \frac{1}{\tilde{E}_n'} \left\{ \hat{D}_{n-2}\tilde{R}_{n-2}'/(1-\tilde{R}_{n-2}') \right.$$
$$\left. +\zeta \hat{D}_{n-1}[\tilde{R}_{n-1}' + (1+\tilde{R}_{n-1}')(S+(1+S)(2R+R^2))]/(1-\tilde{R}_{n-1}') \right\}.$$

Note that $\tilde{R}_n'$ is not yet the calculation $\hat{R}_n'$ of R_n', since in $\hat{R}_n'$ also all operations have to be replaced by their corresponding machine approximations, ζ has to be replaced by $\hat{\zeta}$, and R, S – if not representable – have to be replaced by $\hat{R}, \hat{S}$.

Corollary F.3 *Under the assumptions of Proposition F.1,* $|r_n| \leq R_n \leq \tilde{R}'_n$ *for all* $n \in \mathbf{N}$ *for which* $\tilde{R}'_n$ *is defined.*

PROOF. As in Corollary F.2, the first inequality $|r_n| \leq R_n$ follows from Proposition F.1. The second inequality $R_n \leq \tilde{R}'_n$ follows from the following induction. When $n = 0, 1$, then $R_n \leq \tilde{R}'_n$ since by definition $\tilde{R}'_n = R_n$. Now let $n \geq 2$ and assume that $\tilde{R}'_n$ is defined. By definition of r_i,

$$D_i(1 + r_i) = \hat{D}_i. \tag{F.7}$$

Let $i \in \{n-1, n-2\}$. We have $|r_i| \leq R_i \leq \tilde{R}'_i < 1$, where the last two inequalities hold by induction hypothesis. Hence $|r_i| < 1$, so that in (F.7) we can divide by $1 + r_i$ to give

$$D_i = \hat{D}_i/(1 + r_i).$$

Hence, using that $|r_i| \leq \tilde{R}'_i < 1$,

$$\hat{D}_i/(1 + \tilde{R}'_i) \leq D_i \leq \hat{D}_i/(1 - \tilde{R}'_i). \tag{F.8}$$

The claimed inequality $R_n \leq \tilde{R}'_n$ now follows if in the formula defining R_n we bound D_{n-1} and D_{n-2} according to (F.8), and bound R_{n-1} and R_{n-2} using that by induction hypothesis $R_i \leq \tilde{R}'_i$. **QED**.

The bound R''_n for r_n

By Corollary F.3, the evaluation of the bound R'_n prevents the risk coming from a wrong evaluation of D_n, because if in R'_n one replaces D_n by $\hat{D}_n$ the result is still an upper bound of $|r_n|$, namely $\tilde{R}'_n$. But a numerical evaluation of R'_n involves not only replacing D_n by $\hat{D}_n$, but also replacing all elementary operations in the recursion by their machine approximations (including those needed to calculate ζ). Hence, $\hat{R}'_n$ is not $\tilde{R}'_n$, and we have to ask whether $\hat{R}'_n$ will still be an upper bound of $|r_n|$.

Suppose for a moment that all operations in the recursion defining R'_n or $\tilde{R}'_n$ were well conditioned. Then, as long as n is not extremely large, the accumulated errors would stay moderate, and hence $\hat{R}'_n \approx \tilde{R}'_n (\geq |r_n|)$; if one was disturbed by the "$\approx$", one could instead calculate $2R'_n$, which would certainly yield an upper bound for $|r_n|$.

However, as pointed out in 2. above, the subtraction in the denominator E'_n in R'_n is a possible source of relative error "explosion". In order to tackle this problem, we suggest replacing E'_n by an expression E''_n whose computation

$\hat{E}''_n$ is smaller than $\tilde{E}'_n$, thereby increasing the bound. Specifically, we suggest calculating the following slightly modified bound R''_n. Let $\alpha > 0$ be much smaller than 1, e.g. $\alpha := 10^{-6}$, and define R''_n by the following possibly terminating recursion:

(i) For $n = 0, 1$ put $R''_n := R_n$.

(ii) Let $n \geq 2$. If R''_{n-2} and R''_{n-1} are defined and smaller than α, and in addition

$$E''_n := D_{n-2}(1 - 5R)/(1 + R''_{n-2}) - \zeta D_{n-1}(1 + 2S)(1 + 10R)/(1 - R''_{n-1}) > 0,$$

then R''_n is defined as

$$R''_n := U''_n + (1 + U''_n)(2R + R^2), \tag{F.9}$$

with U''_n depending on D_{n-1}, D_{n-2} and R''_{n-1}, R''_{n-2} via

$$\begin{aligned} U''_n := &\frac{1}{E''_n}\left\{D_{n-2}R''_{n-2}/(1 - R''_{n-2}) + \right. \\ &\left. +\zeta D_{n-1}[R''_{n-1} + (1 + R''_{n-1})(S + (1 + S)(2R + R^2))]/(1 - R''_{n-1})\right\}. \end{aligned} \tag{F.10}$$

Otherwise, R''_n is undefined.

Compared with R'_n, the new denominator E''_n is smaller than E'_n, and hence:

Corollary F.4 *Under the assumptions of Proposition F.1, $|r_n| \leq R_n \leq R'_n \leq R''_n$ for all $n \in \mathbf{N}$ for which R''_n (and hence R'_n) is defined.*

In fact, R''_n is close to R'_n unless there is an error explosion in the denominator, in which case R''_n can become much larger than R'_n. The advantage of R''_n over R'_n lies again in the computation. Consider $\hat{R}'_n$ and $\hat{R}''_n$, the recursively calculated values for R'_n and R''_n, and denote their relative errors *as approximations for* $\tilde{R}'_n$ by q'_n respectively q''_n, viz.

$$\hat{R}'_n = \tilde{R}'_n(1 + q'_n) \quad \text{and} \quad \hat{R}''_n = \tilde{R}'_n(1 + q''_n).$$

While $\hat{R}'_n$ may (in the case of en error explosion in E'_n) be either significantly lower or significantly larger than $\tilde{R}'_n$, we will below argue that, for moderate n, $\hat{R}''_n$ is never significantly lower than $\tilde{R}'_n$, viz.

$$\hat{R}''_n \approx \tilde{R}'_n \quad \text{or} \quad \hat{R}''_n > \tilde{R}'_n. \tag{F.11}$$

Here and in the following, "$\approx$" stands for a (very) small *relative* error q''_n, for instance $|q''_n| \leq 10^{-8}$. In other words, (F.11) means that q''_n is either near 0 or positive – while q'_n is not controlled. We need to assume that the machine accuracy parameters R, S, R_0, R_1 are (very) small, as it is the case in all common software. Also, assume that they are machine representable, so that no $\hat{R}, \hat{S}, \hat{R}_0, \hat{R}_1$ are needed (otherwise use slightly larger bounds that are representable).

The argument why (F.11) holds for moderate n is again by recursion. However, it may happen that (F.11) becomes wrong for very large n (say for $n > 10^4$), since if the recursive argument is applied too often, many small errors in the "wrong direction" may accumulate into a significantly negative q''_n.

For $n = 0, 1$ we have $\hat{R}''_n = \tilde{R}'_n (= R_n)$, so (F.11) is satisfied.

Now let $n \geq 2$ such that $\hat{R}''_n$ is defined, i.e. the recursion is still alive. By induction hypothesis, we have $\hat{R}''_i \approx \tilde{R}'_i$ or $\hat{R}''_i > \tilde{R}'_i$ for $i = n-1, n-2$. Without loss of generality, we may assume that $\hat{R}''_i \approx \tilde{R}'_i$: indeed, if (F.11) holds for $\hat{R}''_i \approx \tilde{R}'_i$ then it also holds when $\hat{R}''_i > \tilde{R}'_i$ (for $i = n-2$ and/or for $i = n-1$) since $\hat{R}''_n$ is larger for larger $\hat{R}''_i$.

Consider $\hat{E}''_n$ and $\hat{U}''_n$, the calculations of E''_n and U''_n. Suppose that we know that

$$\hat{E}''_n \approx \tilde{E}'_n \quad \text{or} \quad \hat{E}''_n < \tilde{E}'_n. \tag{F.12}$$

All operations occurring in (F.10) are numerically stable, where the differences $1 - \hat{R}''_{n-1}$ and $1 - \hat{R}''_{n-2}$ are stable because $\hat{R}''_{n-1}, \hat{R}''_{n-2} < \alpha$ by (ii). Using this and combining with (F.12) and with $\hat{R}''_i \approx R'_i$ for $i = n-1, n-2$, we deduce that

$$\hat{U}''_n \approx \tilde{U}'_n \quad \text{or} \quad \hat{U}''_n < \tilde{U}'_n. \tag{F.13}$$

Now, (F.11) follows by using (F.13) and the fact that all operations in (F.9) are again numerically stable.

So, it remains to show (F.12). The calculation $\hat{E}''_n$ of E''_n can be written as

$$\begin{aligned}\hat{E}''_n = \Big\{ &\Big[\hat{D}_{n-2}(1-5R)/(1+\tilde{R}'_{n-2})\Big](1+s) \\ &- \Big[\zeta\hat{D}_{n-1}(1+10R)(1+2S)/(1-\tilde{R}'_{n-1})\Big](1+s')\Big\}(1+s''),\end{aligned} \tag{F.14}$$

where

- s is the relative error in the calculation of $\hat{D}_{n-2}(1-5R)/(1+\hat{R}''_{n-2})$, but seen as an approximation of $\hat{D}_{n-2}(1-5R)/(1+\tilde{R}'_{n-2})$,

- s' is the relative error in the calculation of $\zeta \hat{D}_{n-1}(1+10R)(1+2S)/(1-\hat{R}''_{n-1})$, but seen as an approximation of $\hat{D}_{n-2}(1-5R)/(1+\tilde{R}'_{n-2})$,
- s'' is the relative error from subtracting the latter result from the former result.

We first treat s, for which we can write

$$1+s = (1+s_1)(1+s_2)(1+s_3)(1+s_4), \tag{F.15}$$

where s_1 is the relative error in $\widehat{1-5R}$, s_2 is the relative error in $\widehat{1+\hat{R}''_{n-2}}$ seen as an approximation of $1+\tilde{R}'_{n-2}$, s_3 is the relative error from multiplying $\hat{D}_{n-2}$ with $\widehat{1-5R}$, and s_4 is the relative error from the division.

Since s_3, s_4 each come from a single operation, we have $|s_3|,|s_4| \leq R$.

The error s_1 comes from calculating $5R$ and subtracting the result $\widehat{5R}$ from 1; as one easily verifies, since $5R$ is very small, s_1 essentially equals the subtraction error, while the effect of the error in $\widehat{5R}$ is negligible; hence in particular $|s_1| < 4R/3$.

Regarding s_2, the argument is as for s_1: this error results from the by induction hypothesis accurate approximation of $\hat{R}''_{n-2}$ by $\tilde{R}''_{n-2}$ and from the addition error; again, s_2 essentially equals the addition error, because $\hat{R}''_{n-2}$ is very small compared to 1 by (ii) in the definition of R''_n; hence in particular $|s_2| \leq 4R/3$.

By the bounds just derived for $r_1, r_2, r_3, r_4,$, the relation (F.15) implies that

$$1+s \leq (1+4R/3)(1+4R/3)(1+R)(1+R) = 1+14R/3+O(R^2) \quad \text{as } R \downarrow 0.$$

In particular, since R is close 0, we have $1+s \leq 1+5R$, and hence in (F.14) we find:

$$\begin{aligned} &\left[\hat{D}_{n-2}(1-5R)/(1+\tilde{R}'_{n-2})\right](1+s) \\ &\leq \hat{D}_{n-2}(1-(5R)^2)/(1+\tilde{R}'_{n-2}) \leq \hat{D}_{n-2}/(1+\tilde{R}'_{n-2}), \end{aligned} \tag{F.16}$$

where this upper bound is precisely the first summand of $\tilde{E}'_n$.

By a very similar procedure for the relative error s', the second term in (F.14) can be bounded below by the second summand in $\tilde{E}'_n$:

$$\left[\zeta \hat{D}_{n-1}(1+10R)(1+2S)/(1-R''_{n-1})\right](1+s') \geq \zeta \hat{D}_{n-1}/(1-\tilde{R}'_{n-1}). \tag{F.17}$$

(The factor $1+2S$ was needed to offset the error in evaluating the square root in ζ.)

By combining the two inequalities (F.16) and (F.17), we can bound $\hat{E}''_n$ (as given by (F.14)) in terms of $\tilde{E}'_n$:

$$\hat{E}''_n \leq \tilde{E}'_n(1+s''),$$

which implies (F.12). **QED**.

Correction for error accumulation

We have shown that the computation of R''_n satisfies $\hat{R}''_n \approx \tilde{R}'_n$ or $\hat{R}''_n > \tilde{R}'_n$, as long as n is moderately large, say $n \leq 10^4$. Other values of n are not needed to calculate $F_\kappa(z)$ (unless $z \to -\infty$). Since $|r_n| \leq \tilde{R}'_n$ by Corollary F.3, we have $|r_n| \approx \hat{R}''_n$ or $|r_n| < \hat{R}''_n$ for moderate n. Only in the unlikely event that rounding errors consistently happen in a way that makes $\hat{R}''_n$ small, $\hat{R}''_n$ may be slightly smaller than $|r_n|$ (for very large n even significantly smaller). To make sure to have calculated an upper bound of $|r_n|$, it is advisable to increase the bound and use, say, the double $2R''_n$. Indeed, the calculation $\widehat{2R''_n} \approx 2\hat{R}''_n$ is then certainly an upper bound for $|r_n|$ for moderate n. If $|r_n|$ has to be bounded for extremely large n, one might multiply R''_n by a factor growing with n, say use the quantity $(2+10^{-4}n)R''_n$ whose calculation should be an upper bound of $|r_n|$ for all n (until the recursion terminates).

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