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NEW FORMULAE FOR HIGHER ORDER DERIVATIVES AND A NEW ALGORITHM FOR NUMERICAL INTEGRATION

by

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Abstract

This thesis is concerned with the development of new formulae for higher order derivatives, and the algorithmic, numerical, and analytical development of the $G_n^{(1)}$ transformation, a method for computing infinite-range integrals. We introduce the Slevinsky-Safouhi formulae I and II with applications, we develop an algorithm for the $G_n^{(1)}$ transformation, we derive explicit approximations to incomplete Bessel functions and tail probabilities of five probability distributions from the recursive algorithm for the $G_n^{(1)}(x)$ transformation, and we present all extant work on the analysis of the convergence properties of the $G_n^{(1)}$ transformation.

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Chapter 1

Introduction

In numerical analysis, in applied mathematics and in physics, infinite series and infinite range integrals represent solutions of many problems. In practice, these series and integrals have a very poor convergence, presenting severe numerical and computational difficulties. As a result, convergence accelerators and nonlinear transformation methods for accelerating the convergence of infinite series and integrals have been studied for many years and have been applied in various situations. They are based on the idea of extrapolation. Via sequence transformations, slowly convergent and divergent sequences and series can be transformed into sequences and series with better numerical properties. Thus, they are useful for accelerating convergence. In the case of nonlinear transformations the improvement of convergence can be remarkable [1–6].

There are numerous applications in science and engineering for special functions and their higher order derivatives. As an example, accurate and fast calculation of highly oscillatory integrals requires reliable extrapolation methods. Examples of such integrals are the Twisted Tail proposed as a computational problem in the SIAM 100-Digit Challenge [7] and the challenging spherical

Bessel integrals involved in the so-called molecular integrals over exponential type functions [8–10] and in integrals of magnetic properties of molecules [11]. The nonlinear D and G transformations [12, 13] have proven to be very powerful tools in the computation of molecular integrals [14–19] and the Twisted Tail [20]. Moreover, the algorithms of these transformations require successive derivatives of the integrands, which can be a severe computational impediment. In highly oscillatory integrands, special functions, like spherical and reduced Bessel functions are prevalent.

In chapter 2, we present new analytic formulae that allow for the calculation of higher order derivatives. These formulae are applicable to functions $G(x)$ for which the terms $\left(\frac{\mathrm{d}}{x^m \mathrm{d}x}\right)^k (x^{-n} G(x))$ for some $m, n \in \mathbb{C}$ are well-defined and easy to compute. The formulae represent the k^{th} derivative as discrete sums of $k + 1$ of the aforementioned terms. The terms in the summation have coefficients that can be computed recursively and are not subject to any computational instability.

Numerically speaking, the analytical development of new formulae is *critical*. As an example, the straightforward calculation of $\left.\frac{\mathrm{d}^{14}}{\mathrm{d}x^{14}} j_n(vx)\right|_{(n,v,x)=(1,1,1)}$ using Maple 11's evalf command to 15 correct digits yields -0.052008. There are two problems with this output: firstly, there are only five significant digits, when 15 are demanded; secondly, the number is only accurate to one digit, the true value being -0.050439 90765 19013. In this case, an accuracy of 28 digits in Maple 11's evalf command is required in order to obtain the exact value to 15 correct digits.

The evaluation of tail integrals of probability distributions is a problem that arises in several fields such as statistics, chemistry and physics. For example, in certain types of clustering and reliability problems, it is required to compute extreme tail probabilities to a high accuracy [21]. Standard quadrature rules had failed to provide extremely accurate computation of tail probabilities leading to the need for approximation functions that yield adequate accuracy for probabilities in the range of interest. Unfortunately, as explained by Gray and Wang [22] there are few general methodologies for producing such functions.

Work in [19, 20] has shown that the $G_n^{(m)}$ transformation [13] can be exceptionally accurate in the computation of highly oscillatory integrals. The G transformation was introduced in [23] and is extended to G_n in [24] and to $G_n^{(m)}$ in [13]. The positive integer m denotes the order of the linear homogeneous differential equation satisfied by the integrand and the positive integer n stands for the truncation order of the asymptotic expansion used in the transformation. The $G_n^{(m)}$ transformation produces approximations to infinite range integrals by expanding the integral tails in asymptotic expansions. One of the main challenges facing the $G_n^{(m)}$ transformation is the lack of efficient algorithms for its implementation. Brute force methods rely on the solution of large systems of linear equations involving successive derivation of the integrands, and are therefore algorithmically undesirable.

In chapter 3, we introduce the $G_n^{(m)}$ transformation, and after outlining its main computational drawbacks, we introduce the recent progress in [25], where a highly efficient algorithm for the implementation of the $G_n^{(1)}$ transformation, for integrals whose integrands satisfy first order linear homogeneous differential equations is introduced. The algorithm requires computation of derivatives of the form $\left(x^2 \frac{\mathrm{d}}{\mathrm{d}x}\right)^n \left(x^{-\nu} f(x)\right)$, where ν is some numerical parameter and where $f(x)$ is either the integrand or its multiplicative inverse.

In chapter 4, we use the algorithm for the $G_n^{(1)}$ transformation introduced in [25] to compute incomplete Bessel functions and the tail probabilities of five probability distributions, namely the normal distribution, the gamma distribution, the student's t-distribution, the inverse Gaussian distribution and Fisher's F distribution. Tail probabilities of the aforementioned five probability distributions are computed and the numerical tables illustrate the high efficiency of the algorithm, which does not resort to any classical numerical integration, such as a quadrature routine. The numerical tables we produce replicate the values treated in [26] with an accuracy reaching as high as 15 correct digits in double precision arithmetic. In addition, some tables show new computations resulting from different values of the parameters in question.

In chapter 5, we study the convergence properties of the $G_n^{(1)}$ transformation. For special yet general forms of integrands, asymptotic error estimates are given, and the rational forms of the approximants are studied. Thus a connection is drawn between the $G_n^{(1)}$ transformation and rational and Padé approximants with an accuracy-through-order condition as well. With this connection established, we identify a correspondence with continued fractions, and it is in the framework of continued fractions that the convergence of the $G_n^{(1)}$ transformation is most easily proved.

Chapter 2

New Formulae For Higher Order Derivatives And Applications

We present new formulae for the analytical development of higher order derivatives. These formulae, which are analytic and exact, represent the k^{th} derivative as a discrete sum of only $k+1$ terms. Involved in the expression for the k^{th} derivative are coefficients of the terms in the summation. These coefficients can be computed recursively and they are not subject to any computational instability. As examples of applications, we develop higher order derivatives of Legendre functions, Chebyshev polynomials of the first kind, Hermite functions and Bessel functions. We also show the general classes of functions to which our new formula is applicable and show how our formula can be applied to certain classes of differential equations.

2.A Existing higher order differentiation formulae

For completeness, we compile a few of the most important higher order differentiation formulae and we refer the interested reader to [27] for other differentiation formulae.

Formula 2.0.1 (The Leibniz Formula): For a function $f(x) = g(x)h(x)$, the derivatives of $f(x)$ can be represented as a sum of derivatives of $g(x)$ and $h(x)$ as:

$$f^{(k)}(x) = \sum_{n=0}^{k} \binom{k}{n} g^{(n)}(x)h^{(k-n)}(x), \tag{2.1}$$

where $\binom{k}{n}$ are the binomial coefficients.

Next, we have a variant of the Leibniz formula for a quotient of two functions. This is not the usual method for defining this higher order derivative; however, this form is computationally efficient.

Formula 2.0.2 (The Quotient Formula): For a function $f(x) = \dfrac{g(x)}{h(x)}$, the derivatives of $f(x)$ can be represented as a sum of derivatives of $g(x)$ and $h(x)$ and lower order derivatives of $f(x)$ as:

$$f^{(k)}(x) = \frac{g^{(k)}(x) - \displaystyle\sum_{n=0}^{k-1} \binom{k}{n} f^{(n)}(x)h^{(k-n)}(x)}{h(x)}. \tag{2.2}$$

Often in the study of nonlinear transformations, linear homogeneous differential equations satisfied by the integrands are generated and studied. The next formula, also a variant of the Leibniz formula, solves for the higher order derivatives of a function satisfying a linear homogeneous differential equation.

Formula 2.0.3 (The Differential Equation Formula): Let $f(x)$ be a function satisfying a differential equation of the form:

$$f^{(m)}(x) = \sum_{k=0}^{m-1} p_k(x) f^{(k)}(x).$$

The derivatives of $f(x)$ can be represented as:

$$f^{(m+n)}(x) = \sum_{k=0}^{m-1} \sum_{i=0}^{n} \binom{n}{i} p_k^{(i)}(x) f^{(k+n-i)}(x), \tag{2.3}$$

where the derivatives $f^{(k)}(x)$ for $k = 1, \ldots, m$ are assumed to be already known.

We also give Faà di Bruno's formula for the higher order derivatives of the chain rule.

Formula 2.0.4 (Faà di Bruno's Formula [28–30]): For a function $f(g(x))$:

$$\frac{\mathrm{d}^n}{\mathrm{d}x^n} f(g(x)) = \sum n! f^{(k)}(g(x)) \prod_{i=1}^{n} \frac{1}{k_i!} \left(\frac{g^{(i)}(x)}{i!} \right)^{k_i}, \tag{2.4}$$

where the summation is over all non-negative integer solutions of the Diophantine equation (2.5) and where k is the count of all non-zero k_i's involved in:

$$\sum_{i=1}^{n} i\, k_i = n. \tag{2.5}$$

2.B New formula for higher order derivatives

In the following theorem, we introduce the Slevinsky-Safouhi Formula I (SSF I) for higher order derivatives.

Theorem 2.1: *Let* $G(x) \in \mathcal{C}^k$ *with the term* $\left(\frac{\mathrm{d}}{x^m \mathrm{d}x}\right)^k (x^{-n} G(x))$ *well-defined and easy to compute for* $m, n \in \mathbb{C}$. *For* $\mu, \nu \in \mathbb{C}$, *the term* $\left(\frac{\mathrm{d}}{x^\mu \mathrm{d}x}\right)^k (x^{-\nu} G(x))$ *is given by:*

$$\left(\frac{\mathrm{d}}{x^\mu \mathrm{d}x}\right)^k (x^{-\nu} G(x)) = \sum_{i=0}^{k} A_k^i \, x^{n-\nu+i(m+1)-k(\mu+1)} \left(\frac{\mathrm{d}}{x^m \mathrm{d}x}\right)^i (x^{-n} G(x)), \tag{2.6}$$

with coefficients:

$$A_k^i = \begin{cases} 1 & \text{for } i = k, \\ (n - \nu - (k-1)(\mu+1)) A_{k-1}^0 & \text{for } i = 0, \ k > 0, \\ (n - \nu + i(m+1) - (k-1)(\mu+1)) A_{k-1}^i + A_{k-1}^{i-1} & \text{for } 0 < i < k. \end{cases} \tag{2.7}$$

Moreover, for $m \neq -1$, *these coefficients have the explicit expression:*

$$A_k^i = \sum_{j=0}^{i} \frac{(-1)^{i-j} \, (n - \nu + j(m+1) - (k-1)(\mu+1))_{k,\mu+1}}{(m+1)^i \, j! \, (i-j)!}, \tag{2.8}$$

where $(x)_{n,k}$ *is the Pochhammer* k*-symbol [31] and can be computed as* $\prod_{l=0}^{n-1} (x + kl)$.

Proof. It is easy to show that equation (2.6) holds for $k = 0$, since:

$$x^{-\nu} \, G(x) = x^{n-\nu} (x^{-n} \, G(x)). \tag{2.9}$$

For $k = 1$, we show that equations (2.6) and (2.7) hold by applying $\left(\frac{\mathrm{d}}{x^\mu \mathrm{d}x}\right)$ to both sides of (2.9):

$$\left(\frac{\mathrm{d}}{x^\mu \mathrm{d}x}\right)(x^{-\nu}G(x)) = (n-\nu)\, x^{n-\nu-\mu-1}(x^{-n}G(x)) + x^{n-\nu+m-\mu}\left(\frac{\mathrm{d}}{x^m \mathrm{d}x}\right)(x^{-n}G(x)). \tag{2.10}$$

As (2.6) and (2.7) are true for $k = 0, 1$, we now assume they hold for $k-1$:

$$\left(\frac{\mathrm{d}}{x^\mu \mathrm{d}x}\right)^{k-1}(x^{-\nu}G(x)) = \sum_{i=0}^{k-1} A_{k-1}^i\, x^{n-\nu+i(m+1)-(k-1)(\mu+1)}\left(\frac{\mathrm{d}}{x^m \mathrm{d}x}\right)^i (x^{-n}G(x)). \tag{2.11}$$

Applying the correct operator to both sides of the equation yields:

$$\begin{aligned}\left(\frac{\mathrm{d}}{x^\mu \mathrm{d}x}\right)^{k}(x^{-\nu}G(x)) &= \frac{\mathrm{d}}{x^\mu \mathrm{d}x}\sum_{i=0}^{k-1} A_{k-1}^i\, x^{n-\nu+i(m+1)-(k-1)(\mu+1)}\left(\frac{\mathrm{d}}{x^m \mathrm{d}x}\right)^i (x^{-n}G(x)) \\ = \sum_{i=0}^{k-1} A_{k-1}^i \Bigg[&(n-\nu+i(m+1)-(k-1)(\mu+1))\, x^{n-\nu+i(m+1)-k(\mu+1)}\left(\frac{\mathrm{d}}{x^m \mathrm{d}x}\right)^i (x^{-n}G(x)) \\ + x^{n-\nu+(i+1)(m+1)-k(\mu+1)}&\left(\frac{\mathrm{d}}{x^m \mathrm{d}x}\right)^{i+1}(x^{-n}G(x))\Bigg].\end{aligned} \tag{2.12}$$

Explicitly grouping equal powers of terms $x^{n-\nu+i(m+1)-k(\mu+1)}\left(\frac{\mathrm{d}}{x^m \mathrm{d}x}\right)^i (x^{-n}G(x))$ in the series gives:

$$\left(\frac{\mathrm{d}}{x^\mu \mathrm{d}x}\right)^{k}(x^{-\nu}G(x)) = (n-\nu-(k-1)(\mu+1))A_{k-1}^0\, x^{n-\nu-k(\mu+1)}(x^{-n}G(x)) \tag{2.13}$$

$$\begin{aligned}&+\sum_{i=1}^{k-1}\left[(n-\nu+i(m+1)-(k-1)(\mu+1))A_{k-1}^i + A_{k-1}^{i-1}\right] x^{n-\nu+i(m+1)-k(\mu+1)}\left(\frac{\mathrm{d}}{x^m \mathrm{d}x}\right)^i (x^{-n}G(x)) \\ &+ A_{k-1}^{k-1}\, x^{n-\nu+k(m-\mu)}\left(\frac{\mathrm{d}}{x^m \mathrm{d}x}\right)^k (x^{-n}G(x)),\end{aligned} \tag{2.14}$$

which recovers the recurrence relations for the coefficients in (2.7).

To prove the explicit expression (2.8), consider the main recurrence relation:

$$A_k^i = (n - \nu + i(m+1) - (k-1)(\mu+1))A_{k-1}^i + A_{k-1}^{i-1}, \tag{2.15}$$

and consider the triangular nature of the coefficients A_k^i, with values $0 \le i \le k$, $k \ge 0$.

We begin by defining the auxiliary coefficients:

$$D_k^i = (n - \nu + i(m+1) - (k-1)(\mu+1))D_{k-1}^i \qquad \text{and} \qquad D_0^i = 1, \tag{2.16}$$

that have the simple explicit solution:

$$D_k^i = (n - \nu + i(m+1) - (k-1)(\mu+1))_{k,\mu+1}. \tag{2.17}$$

Naturally, $D_k^0 = A_k^0$. In addition:

$$\begin{cases} D_k^1 = (m+1)\, A_k^1 + A_k^0 = (m+1)\, A_k^1 + D_k^0 \\ D_k^2 = 2(m+1)^2\, A_k^2 + 2(m+1)A_k^1 + A_k^0 = 2\,(m+1)^2\, A_k^2 + 2\, D_k^1 - D_k^0, \end{cases} \tag{2.18}$$

and in general:

$$D_k^i = i!\,(m+1)^i\, A_k^i + \sum_{j=0}^{i-1} \binom{i}{j} (-1)^{i-1-j}\, D_k^j, \tag{2.19}$$

which ultimately leads to:

$$A_k^i = \sum_{j=0}^{i} \frac{(-1)^{i-j}\, D_k^j}{(m+1)^i\, j!\,(i-j)!}, \tag{2.20}$$

whereupon the explicit expression for the coefficients is easily deduced. For

$m = -1$, we note that $D_k^0 = D_k^1 = \cdots = D_k^k$. Therefore, we do not have i independent auxiliary coefficients D_k^i from which to form a linear combination representation for A_k^i. $\square$

The case $(\mu, \nu, m, n) = (0, 0, 1, 0)$ appears so often that we have the following Corollary:

Corollary 2.1.1 (The SSF II): Let $G(x) \in \mathcal{C}^k$ with the term $\left(\frac{\mathrm{d}}{x\mathrm{d}x}\right)^k G(x)$ well-defined and easy to compute. The term $\frac{\mathrm{d}^k G}{\mathrm{d}x^k}$ is given by:

$$\frac{\mathrm{d}^k G}{\mathrm{d}x^k} = \sum_{i=\lfloor\frac{k+1}{2}\rfloor}^{k} \hat{A}_k^i \, x^{2i-k} \left(\frac{\mathrm{d}}{x\mathrm{d}x}\right)^i G(x), \tag{2.21}$$

with coefficients:

$$\hat{A}_k^i = \begin{cases} 1 & \text{for } i = k \\ 2\,\hat{A}_{k-1}^i + \hat{A}_{k-1}^{i-1} & \text{for } i = \lfloor\frac{k+1}{2}\rfloor,\ k \text{ odd} \\ \hat{A}_{k-1}^i & \text{for } i = \lfloor\frac{k+1}{2}\rfloor,\ k \text{ even} \\ (2i-k+1)\hat{A}_{k-1}^i + \hat{A}_{k-1}^{i-1} & \text{for } \lfloor\frac{k+1}{2}\rfloor < i < k,\ k > 3, \end{cases} \tag{2.22}$$

where $\lfloor\alpha\rfloor$ is the integer floor function of argument α.

Moreover, these coefficients have the explicit expression:

$$\hat{A}_k^i = \sum_{j=0}^{i} \frac{(-1)^{i-j}(2j-k+1)_k}{2^i\, j!\,(i-j)!}, \tag{2.23}$$

where $(x)_n$ is the Pochhammer symbol.

Although analytical formulae for the coefficients A_k^i and $\hat{A}_k^i$ are of importance, the recurrence relations also have their own advantages. The analytical formulae are very useful when only a single derivative of high order is required, whereas from a numerical and/or computational perspective, recurrence relations are more efficient when evaluating a sequence of derivatives.

2.B.1 The generality

With no loss of generality, Theorem 2.1 with $(\mu, \nu, m, n) = (0, 0, m, n)$ can formulate the k^{th} derivative of any function $G(x) = x^n\, f(x^{m+1})$, since:

$$\left(\frac{\mathrm{d}}{x^m \mathrm{d}x}\right)^i (x^{-n}\, G(x)) = \left(\frac{\mathrm{d}}{x^m \mathrm{d}x}\right)^i f(x^{m+1}) = (m+1)^i\, f^{(i)}(x^{m+1}), \qquad (2.24)$$

where $f^{(i)}(x^{m+1})$ stands for the derivative of f with respect to its argument. It follows that:

$$\frac{\mathrm{d}^k}{\mathrm{d}x^k}(x^n f(x^{m+1})) = \sum_{i=0}^{k} A_k^i\, x^{n+i(m+1)-k}(m+1)^i\, f^{(i)}(x^{m+1}), \qquad (2.25)$$

with coefficients A_k^i given by (2.7). Higher order derivatives of $f(x^{m+1})$ are developed in [27], and we present the formula here for comparison with (2.25):

$$\frac{\mathrm{d}^k}{\mathrm{d}x^k} f(x^{m+1}) = \sum_{i=0}^{k} \sum_{j=0}^{i} \frac{(-1)^j((m+1)(i-j)-k+1)_k\, f^{(i)}(x^{m+1})}{j!\,(i-j)!\, x^{k-i(m+1)}}. \qquad (2.26)$$

Equations (2.25) and (2.26) are very similar in form and it is easy to show that (2.26) is a specific case of Theorem 2.1. Note that the case $m = -1$ in (2.25) realizes a power function $G(x) = x^n f(1)$.

However, the case $m = -1$ extends naturally to functions $G(x) = x^n f(\ln(x))$, since:

$$\left(x\frac{\mathrm{d}}{\mathrm{d}x}\right)^i (x^{-n}\, G(x)) = \left(x\frac{\mathrm{d}}{\mathrm{d}x}\right)^i f(\ln(x)) = f^{(i)}(\ln(x)), \qquad (2.27)$$

where $f^{(i)}(\ln(x))$ stands for the derivative of f with respect to its argument. It follows that:

$$\frac{\mathrm{d}^k}{\mathrm{d}x^k}(x^n f(\ln(x))) = \sum_{i=0}^{k} A_k^i \, x^{n-k} f^{(i)}(\ln(x)), \tag{2.28}$$

with coefficients A_k^i given by (2.7).

It is worth noting that higher order derivatives of $f(\ln(x))$ are given in the book [32] as:

$$\frac{\mathrm{d}^k}{\mathrm{d}x^k} f(\ln(x)) = \frac{1}{x^k} \sum_{i=1}^{k} (-1)^{k-i} \begin{bmatrix} k \\ i \end{bmatrix} f^{(i)}(\ln(x)), \tag{2.29}$$

where $\begin{bmatrix} k \\ i \end{bmatrix}$ are the Stirling numbers of the first kind. Thus formula (2.28) follows at once from (2.29) and the Leibniz formula.

Lastly, by performing the substitution $x \leftrightarrow e^x$ in (2.6) with $(\mu, \nu, m, n) = (-1, 0, 0, n)$, we obtain for the functions $G(x) = e^{n\,x} f(e^x)$:

$$\frac{\mathrm{d}^k}{\mathrm{d}x^k}(e^{n\,x} f(e^x)) = \sum_{i=0}^{k} A_k^i \, e^{(n+i)x} f^{(i)}(e^x), \tag{2.30}$$

with coefficients A_k^i given by (2.7), which again follows at once from:

$$\frac{\mathrm{d}^k}{\mathrm{d}x^k} f(e^x) = \sum_{i=1}^{k} \begin{Bmatrix} k \\ i \end{Bmatrix} e^{i\,x} f^{(i)}(e^x), \tag{2.31}$$

found in the book [32] and the Leibniz formula. Here, $\begin{Bmatrix} k \\ i \end{Bmatrix}$ are the Stirling numbers of the second kind.

Interestingly, these two developments show how Stirling numbers of both the first and the second kinds are specific cases of the coefficients A_k^i. Explicitly, Stirling numbers of the first kind are given by coefficients A_k^i with $(\mu, \nu, m, n) = (0, 0, -1, 0)$, and Stirling numbers of the second kind are given by coefficients A_k^i with $(\mu, \nu, m, n) = (-1, 0, 0, 0)$.

Remark: This section illustrates the connection between Theorem 2.1 and Faà di Bruno's formula (Formula 2.0.4) for $\frac{\mathrm{d}^k}{\mathrm{d}x^k} f(g(x))$, which has been recently applied in the numerical evaluation of a challenging integral [20]. In approaching the general composition $f(g(x))$, we would naturally represent its derivatives as a linear combination of operators $\left(\frac{\mathrm{d}}{g'(x)\mathrm{d}x}\right)^k f(g(x)) = f^{(k)}(g(x))$. Indeed, the aforementioned representation forms the heart of Hoppe's Formula [30, 33–35]:

Formula 2.1.1 (Hoppe's Formula): For functions f and g sufficiently differentiable:

$$\frac{\mathrm{d}^k}{\mathrm{d}x^k} f(g(x)) = \sum_{i=0}^{k} \tilde{A}_k^i(x)\, f^{(i)}(g(x)), \tag{2.32}$$

where:

$$\tilde{A}_k^i(x) = \sum_{j=0}^{i} \frac{(-1)^{i-j}}{j!\,(i-j)!} (g(x))^{i-j} \frac{\mathrm{d}^k}{\mathrm{d}x^k} (g(x))^j. \tag{2.33}$$

It is mentioned in [30] that the functions $\tilde{A}_k^i(x)$ satisfy:

$$\tilde{A}_k^i(x) = \frac{\mathrm{d}}{\mathrm{d}x} \tilde{A}_{k-1}^i(x) + g'(x)\, \tilde{A}_{k-1}^{i-1}(x), \tag{2.34}$$

a result that can easily prove the formula by induction.

Hoppe's formula is generally regarded as an unsatisfactory solution to the chain rule problem, as it simply reduces the exterior function f to a power function in (2.33). With today's symbolic programming languages, equation (2.34) could easily be used to create a significantly faster code for the higher order derivatives of the chain rule than can be created by Faà di Bruno's formula (Formula 2.0.4).

2.B.2 Properties of the coefficients

In this section, we provide a number of properties satisfied by the coefficients A_k^i of the SSF I. The fundamental aspect of these coefficients is that they satisfy the recurrence relation (2.7):

$$A_k^i = (n - \nu + i(m+1) - (k-1)(\mu+1))A_{k-1}^i + A_{k-1}^{i-1}, \qquad A_0^0 = 1.$$

Matrix properties

Proposition 2.1: *Let A_k^i represent the coefficients in (2.7) for $\mu, \nu, m, n \in \mathbb{C}$ and where necessary, let $A_k^i(\mu, \nu, m, n)$ represent those same coefficients. Let $\mathbf{A}$ denote the $k+1 \times k+1$ lower triangular matrix:*

$$\mathbf{A} = \begin{bmatrix} A_0^0 & & & & 0 \\ A_1^0 & A_1^1 & & & \\ A_2^0 & A_2^1 & \ddots & & \\ \vdots & \vdots & \ddots & \ddots & \\ A_k^0 & A_k^1 & \cdots & A_k^{k-1} & A_k^k \end{bmatrix}, \tag{2.35}$$

of coefficients A_k^i and where necessary, let $\mathbf{A}_{\mu\nu}^{mn}$ denote the matrix of $A_k^i(\mu, \nu, m, n)$. The following properties hold:

1. $\det \mathbf{A} = 1$*;*

2. $\left(\mathbf{A}_{\mu\nu}^{mn}\right)^{-1} = \mathbf{A}_{mn}^{\mu\nu}$ *and consequently,* $\mathbf{A}_{\mu\nu}^{mn}\mathbf{A}_{mn}^{\mu\nu} = \mathbf{A}_{mn}^{\mu\nu}\mathbf{A}_{\mu\nu}^{mn} = \mathbf{I}$*;*

3. $\displaystyle\sum_{k=0}^{\max\{i,j\}} A_k^i(\mu,\nu,m,n)A_j^k(m,n,\mu,\nu) = \delta_{ij}$; *and,*

4. $\displaystyle\sum_{k=0}^{\max\{i,j\}} A_k^i(m,n,\mu,\nu)A_j^k(\mu,\nu,m,n) = \delta_{ij}$.

Proof. From the recurrence relation for the coefficients A_k^i, the diagonal elements of $\mathbf{A}$ are all 1, and since the determinant of the triangular matrix (2.35) is $\displaystyle\prod_{i=0}^{k} A_i^i$, we retrieve property 1. To prove property 2, let the $k+1 \times 1$ column vectors $\mathbf{\Gamma}$ and $\mathbf{G}$ denote:

$$\mathbf{\Gamma} = \begin{bmatrix} G \\ x^{\nu+(\mu+1)}\left(\frac{\mathrm{d}}{x^{\mu}\mathrm{d}x}\right)(x^{-\nu}G) \\ \vdots \\ x^{\nu+k(\mu+1)}\left(\frac{\mathrm{d}}{x^{\mu}\mathrm{d}x}\right)^k(x^{-\nu}G) \end{bmatrix} \quad \text{and} \quad \mathbf{G} = \begin{bmatrix} G \\ x^{n+(m+1)}\left(\frac{\mathrm{d}}{x^{m}\mathrm{d}x}\right)(x^{-n}G) \\ \vdots \\ x^{n+k(m+1)}\left(\frac{\mathrm{d}}{x^{m}\mathrm{d}x}\right)^k(x^{-n}G) \end{bmatrix}. \tag{2.36}$$

Then, the SSF I in matrix notation is $\mathbf{\Gamma} = \mathbf{A}_{\mu\nu}^{mn}\mathbf{G}$. Inverting this system and solving for $\mathbf{G}$, we obtain $\mathbf{G} = \left(\mathbf{A}_{\mu\nu}^{mn}\right)^{-1}\mathbf{\Gamma}$. However, we also obtain $\mathbf{G} = \mathbf{A}_{mn}^{\mu\nu}\mathbf{\Gamma}$ by the SSF I and equality between both relations proves property 2. Properties 3 and 4 are the explicit $2(k+1)^2$ equations of the multiplication of $\mathbf{A}_{\mu\nu}^{mn}\mathbf{A}_{mn}^{\mu\nu} = \mathbf{A}_{mn}^{\mu\nu}\mathbf{A}_{\mu\nu}^{mn} = \mathbf{I}$. $\square$

Zero array

Proposition 2.2: *Let A_k^i represent the coefficients in* (2.7) *for $\mu,\nu,m,n \in \mathbb{C}$. Let $k_0 = \frac{n-\nu}{\mu+1} + 1$. If $\frac{n-\nu}{\mu+1} \in \mathbb{N}_0$, then $k_0 \in \mathbb{N}$ and therefore:*

$$A_k^0 = 0, \quad \forall k \geq k_0. \tag{2.37}$$

Furthermore, let $k_i = k_{i-1} + \frac{m+1}{\mu+1}$ *for* $i \in \mathbb{N}$*. If* $\frac{m+1}{\mu+1} \in \mathbb{N}$*, then* $k_i \in \mathbb{N}\ \forall i \in \mathbb{N}$ *and therefore given* i*:*

$$A^i_k = 0, \quad \forall k \geq k_i. \tag{2.38}$$

Proof. From the recurrence relation (2.7) for $A^0_{k_0}$:

$$\begin{aligned} A^0_{k_0} &= (n - \nu - (k_0 - 1)(\mu + 1))A^0_{k_0-1}, &(2.39)\\ &= (n - \nu - \left(\frac{n-\nu}{\mu+1}\right)(\mu + 1))A^0_{k_0-1}, &(2.40)\\ &= (n - \nu - (n - \nu))A^0_{k_0-1}, &(2.41)\\ &= 0. &(2.42)\end{aligned}$$

We consider the recurrence relation (2.7) for $A^i_{k_i}$:

$$A^i_{k_i} = (n - \nu + i(m + 1) - (k_i - 1)(\mu + 1))A^i_{k_i-1} + A^{i-1}_{k_i-1}. \tag{2.43}$$

But the sequence $\{k_i\}_{i\in\mathbb{N}_0}$ is monotonically increasing, so $k_i > k_{i-1}$ implies $A^{i-1}_{k_i-1} = 0$ and so:

$$\begin{aligned} A^i_{k_i} &= (n - \nu + i(m + 1) - \left(\frac{n-\nu+i(m+1)}{\mu+1}\right)(\mu + 1))A^i_{k_i-1} + 0, &(2.44)\\ &= (n - \nu + i(m + 1) - (n - \nu + i(m + 1)))A^i_{k_i-1}, &(2.45)\\ &= 0. &(2.46)\end{aligned}$$

This induction on i proves the result. □

Considering the preceding results, the array A^i_k may contain a zero array as depicted in Figure 2.1.

Remark: The potential occurrence of a zero array in the A^i_k explains why the

$$\begin{array}{ccccc}
A_0^0 & & & & \\
A_1^0 & A_1^1 & & & \\
A_2^0 & A_2^1 & A_2^2 & & \\
A_3^0 & A_3^1 & A_3^2 & A_3^3 & \\
\vdots & \vdots & \vdots & \vdots & \ddots \\
0 & A_{k_0}^1 & A_{k_0}^2 & A_{k_0}^3 & \cdots \\
\vdots & \vdots & \vdots & \vdots & \ddots \\
0 & 0 & A_{k_1}^2 & A_{k_1}^3 & \cdots \\
\vdots & \vdots & \vdots & \vdots & \ddots \\
0 & 0 & 0 & A_{k_2}^3 & \cdots \\
\vdots & \vdots & \vdots & \vdots & \ddots
\end{array}$$

Figure 2.1: The occurrence of a zero array in the coefficients A_k^i.

coefficients $\hat{A}_k^i$ of the SSF II are only defined for $i = \lfloor \frac{k+1}{2} \rfloor, \ldots, k$ and not for $i = 0, \ldots, k$: the coefficients $\hat{A}_k^i$ correspond to the coefficients A_k^i with $(\mu, \nu, m, n) = (0, 0, 1, 0)$. This correspondence implies that the sequence $\{k_i\}$ is given by $k_i = 2\,i + 1$. This sequence provides for a zero array, and therefore summation may invariably begin at the first nonzero element in $\hat{A}_k^i$.

The generating function

Proposition 2.3: *Let A_k^i represent the coefficients in (2.7) for $\mu, \nu, m, n \in \mathbb{C}$. The bivariate generating function for the coefficients A_k^i is given by:*

$$A(x, y) = \sum_{k=0}^{\infty} \sum_{i=0}^{k} A_k^i \frac{x^i\, y^k}{k!\,(\mu+1)^k} = (y+1)^{\frac{n-\nu}{\mu+1}} \exp\left\{ \frac{\left((y+1)^{\frac{m+1}{\mu+1}} - 1\right) x}{m+1} \right\}. \tag{2.47}$$

Consequently:

$$A_k^i = \frac{\partial^{i+k}}{\partial x^i \partial y^k} \frac{A(x,y)(\mu+1)^k}{i!}\Bigg|_{(x,y)=(0,0)}. \tag{2.48}$$

Proof. Multiplying the recurrence relation (2.7) by $\dfrac{x^i\, y^k}{k!\,(\mu+1)^k}$ and summing over i and k, we obtain the partial differential equation:

$$(m+1)\, x\, \frac{\partial A}{\partial x} - (\mu+1)(y+1)\frac{\partial A}{\partial y} = (\nu - n - x)A. \tag{2.49}$$

Employing the method of characteristics, we obtain the general solution:

$$A(x,y) = F((y+1)x^{\frac{\mu+1}{m+1}})x^{\frac{\nu-n}{m+1}}e^{-x/(m+1)}. \tag{2.50}$$

Considering the initial value $A(x,0) = 1$ due to $A_0^0 = 1$, we find that $F(x) = x^{\frac{n-\nu}{\mu+1}} \exp\left(x^{\frac{m+1}{\mu+1}}/(m+1)\right)$. Inserting this function into (2.50), we obtain the closed form expression for the generating function (2.47). It is then trivial to obtain the symbolic expression for the coefficients (2.48). □

Asymptotic forms

Proposition 2.4: *Let A_k^i represent the coefficients in* (2.7) *for $\mu, \nu, m, n \in \mathbb{C}$.*

For $m \neq \mu$, the asymptotic form holds:

$$A_k^{k-i} \sim \zeta(i)\, k^{2i}, \quad \text{as} \quad k \to \infty, \quad i \text{ fixed}, \tag{2.51}$$

where $\zeta(i) = \dfrac{(m-\mu)^i}{2^i\, i!}$, while for $m = \mu$, the asymptotic form holds:

$$A_k^{k-i} \sim \xi(i)\, k^{i}, \quad \text{as} \quad k \to \infty, \quad i \text{ fixed}, \tag{2.52}$$

where $\xi(i) = (m+1)^i \binom{\frac{n-\nu}{m+1}}{i}$.

Proof. Substituting $i \to k-i$ in (2.7), we obtain:

$$A_k^{k-i} = (n - \nu + (k-i)(m+1) - (k-1)(\mu+1))A_{k-1}^{k-i} + A_{k-1}^{k-i-1}, \qquad A_0^0 = 1, \tag{2.53}$$

$$= (n - \nu - (i-1)(m+1) + (k-1)(m-\mu))A_{k-1}^{k-i} + A_{k-1}^{k-i-1}. \tag{2.54}$$

Then, since:

$$A_k^{k-i} - A_{k-1}^{k-i-1} = (n - \nu - (i-1)(m+1) + (k-1)(m-\mu))A_{k-1}^{k-i}, \tag{2.55}$$

the telescoping summation over k gives:

$$\sum_{j=i}^{k} (A_j^{j-i} - A_{j-1}^{j-i-1}) = A_k^{k-i} - A_{i-1}^{-1}, \tag{2.56}$$

$$= A_k^{k-i} = \sum_{j=i}^{k} (n - \nu - (i-1)(m+1) + (j-1)(m-\mu))A_{j-1}^{j-i}. \tag{2.57}$$

Consider now the case $i = 1$, such that:

$$A_k^{k-1} = \sum_{j=1}^{k} (n - \nu + (j-1)(m-\mu))A_{k-1}^{k-1}. \tag{2.58}$$

But $A_{k-1}^{k-1} = 1$, so:

$$A_k^{k-1} = (n-\nu)\sum_{j=1}^{k} 1 + (m-\mu)\sum_{j=1}^{k}(j-1), \tag{2.59}$$

$$= (n-\nu)k + (m-\mu)\left(\frac{k^2-k}{2}\right). \tag{2.60}$$

By induction over i in equation (2.57), the coefficients may be written as:

$$A_k^{k-i} = \prod_{j=1}^{i} \left[(n - \nu - (j-1)(m+1)) f_{i,j}(k) + (m - \mu) g_{i,j}(k) \right], \tag{2.61}$$

for some polynomials $f_{i,j}(k)$ and $g_{i,j}(k)$ in k. For the case where $m \neq \mu$, we rely on $\deg(g_{i,j}(k)) > \deg(f_{i,j}(k))$ to produce the leading asymptotic term of A_k^{k-i}, which is given by $(m-\mu)^i \prod_{j=1}^{i} g_{i,j}(k)$. On comparison of (2.57) and (2.61), the product of the polynomials $g_{i,j}(k)$ is produced from the recurrence:

$$\prod_{j=1}^{i} g_{i,j}(k) = \sum_{j=i}^{k} (j-1) \prod_{l=1}^{i-1} g_{i-1,l}(j), \tag{2.62}$$

whereby the dominant term in this product is $\dfrac{k^{2i}}{2^i\, i!}$ as $k \to \infty$.

For the case where $m = \mu$, the telescoping sum (2.57) reduces to:

$$A_k^{k-i} = \sum_{j=i}^{k} (n - \nu - (i-1)(m+1)) A_{j-1}^{j-i}, \tag{2.63}$$

and the product (2.61) reduces to:

$$A_k^{k-i} = \prod_{j=1}^{i} (n - \nu - (j-1)(m+1)) f_{i,j}(k). \tag{2.64}$$

On comparison of (2.63) and (2.64), the product of the polynomials $f_{i,j}(k)$ is produced from the recurrence:

$$\prod_{j=1}^{i} f_{i,j}(k) = \sum_{j=i}^{k} \prod_{l=1}^{i-1} f_{i-1,l}(j), \tag{2.65}$$

whereby the dominant term in this product is $\dfrac{k^i}{i!}$ as $k \to \infty$. Finally, the product:

$$\prod_{j=1}^{i}(n-\nu-(j-1)(m+1)) = (n-\nu-(i-1)(m+1))_{i,m+1} = i!(m+1)^i\binom{\frac{n-\nu}{m+1}}{i}, \tag{2.66}$$

and by combination, the result is obtained. □

Tables 2.1 and 2.2 illustrate the asymptotic nature of the equations (2.51) and (2.52) to the coefficients A_k^{k-i} for some values of k, i, and μ, ν, m and n.

$k\backslash i$	1	5	8
1	0.33333		
3	0.77778		
10	0.93333	0.04283	0.00004
30	0.97778	0.40463	0.08262
100	0.99333	0.77103	0.49904
300	0.99778	0.91789	0.79669
1000	0.99933	0.97473	0.93450

Table 2.1: Ratio of the coefficients A_k^{k-i} to $\zeta(i)k^{2i}$, the asymptotic term given by (2.51) for $(\mu, \nu, m, n) = (-2, -1/2, 1, 0)$.

$k\backslash i$	1	5	8
1	1.00000		
3	1.00000		
10	1.00000	0.30240	0.01814
30	1.00000	0.70373	0.35969
100	1.00000	0.90345	0.75031
300	1.00000	0.96705	0.91017
1000	1.00000	0.99003	0.97232

Table 2.2: Ratio of the coefficients A_k^{k-i} to $\xi(i)k^i$, the asymptotic term given by (2.52) for $(\mu, \nu, m, n) = (3, 0, 3, 2)$.

2.C Applications

2.C.1 Legendre functions

The importance of higher order derivatives of Legendre functions is discussed in [36]. These aforementioned functions are defined through the Rodrigues formula [37]:

$$P_\ell^m(x) = \frac{(-1)^m}{2^\ell \ell!} \left(1-x^2\right)^{\frac{m}{2}} \frac{\mathrm{d}^{\ell+m}}{\mathrm{d}x^{\ell+m}} \left(x^2-1\right)^\ell . \tag{2.67}$$

Therefore, it is natural with the help of the Leibniz Formula (Formula 2.0.1) to define the higher order derivatives of these functions as:

$$\frac{\mathrm{d}^k}{\mathrm{d}x^k} P_\ell^m(x) = \frac{(-1)^m}{2^\ell\, \ell!} \sum_{n=0}^{k} \binom{k}{n} \frac{\mathrm{d}^n}{\mathrm{d}x^n} \left(1-x^2\right)^{\frac{m}{2}} \frac{\mathrm{d}^{\ell+m+k-n}}{\mathrm{d}x^{\ell+m+k-n}} \left(x^2-1\right)^\ell . \tag{2.68}$$

The problem areas in this formula are the terms $\frac{\mathrm{d}^n}{\mathrm{d}x^n}\left(1-x^2\right)^{\frac{m}{2}}$ and $\frac{\mathrm{d}^{\ell+m+k-n}}{\mathrm{d}x^{\ell+m+k-n}}\left(x^2-1\right)^\ell$.

Considering that the identities:

$$\begin{cases} \left(\dfrac{\mathrm{d}}{x\mathrm{d}x}\right)^i \left(1-x^2\right)^{\frac{m}{2}} = (-2)^i \left(1-x^2\right)^{\frac{m}{2}-i} \displaystyle\prod_{j=0}^{i-1} \left(\frac{m}{2}-j\right) \\ \left(\dfrac{\mathrm{d}}{x\mathrm{d}x}\right)^i \left(x^2-1\right)^\ell \ = 2^i \left(x^2-1\right)^{\ell-i} \displaystyle\prod_{j=0}^{i-1} (\ell-j), \end{cases} \tag{2.69}$$

are computed with exceptional simplicity, we apply the result of Corollary

2.1.1 and develop:

$$\begin{cases} \dfrac{\mathrm{d}^n}{\mathrm{d}x^n}\left(1-x^2\right)^{\frac{m}{2}} = \displaystyle\sum_{i=\lfloor\frac{n+1}{2}\rfloor}^{n} \hat{A}_n^i\, x^{2i-n}\,(-2)^i\,(1-x^2)^{\frac{m}{2}-i}\prod_{j=0}^{i-1}\left(\frac{m}{2}-j\right) \\ \dfrac{\mathrm{d}^{\ell+m+k-n}}{\mathrm{d}x^{\ell+m+k-n}}\left(x^2-1\right)^{\ell} = \displaystyle\sum_{i=\lfloor\frac{\ell+m+k-n+1}{2}\rfloor}^{\ell+m+k-n} \hat{A}_{\ell+m+k-n}^i\, x^{2i-\ell-m-k+n}\,2^i\,(x^2-1)^{\ell-i}\prod_{j=0}^{i-1}(\ell-j), \end{cases} \tag{2.70}$$

with coefficients $\hat{A}_k^i$ given by (2.22). This ultimately leads to the final result:

$$\begin{aligned} \frac{\mathrm{d}^k}{\mathrm{d}x^k}P_\ell^m(x) = \frac{(-1)^m}{2^\ell \ell!}\sum_{n=0}^{k}\binom{k}{n}\Bigg\{&\left[\sum_{i=\lfloor\frac{n+1}{2}\rfloor}^{n}\hat{A}_n^i\, x^{2i-n}(-2)^i(1-x^2)^{\frac{m}{2}-i}\prod_{j=0}^{i-1}\left(\frac{m}{2}-j\right)\right] \\ &\times\left[\sum_{i=\lfloor\frac{\ell+m+k-n+1}{2}\rfloor}^{\ell+m+k-n}\hat{A}_{\ell+m+k-n}^i\, x^{2i-\ell-m-k+n}\,2^i\,(x^2-1)^{\ell-i}\prod_{j=0}^{i-1}(\ell-j)\right]\Bigg\}. \end{aligned} \tag{2.71}$$

In [36], $\dfrac{\mathrm{d}^k}{\mathrm{d}\theta^k}P_\ell^m(\cos(\theta))$ is developed using recurrence relations as:

$$\frac{\mathrm{d}^k}{\mathrm{d}\theta^k}P_\ell^m(\cos(\theta)) = \frac{\mathrm{d}^{k-1}}{\mathrm{d}\theta^{k-1}}P_\ell^{m+1}(\cos(\theta)) - (\ell+m)(\ell-m+1)\frac{\mathrm{d}^{k-1}}{\mathrm{d}\theta^{k-1}}P_\ell^{m-1}(\cos(\theta)), \tag{2.72}$$

and, for Legendre *polynomials*, there is [37]:

$$\frac{\mathrm{d}^k}{\mathrm{d}x^k}P_\ell(x) = \frac{\mathrm{d}^{k-1}}{\mathrm{d}x^{k-1}}P_{\ell-2}(x) + (2\ell-1)\frac{\mathrm{d}^{k-1}}{\mathrm{d}x^{k-1}}P_{\ell-1}(x). \tag{2.73}$$

This simplicity cannot be extended to $\dfrac{\mathrm{d}^k}{\mathrm{d}x^k}P_\ell^m(x)$, as these recurrence relations have non-constant coefficients in x. There also exist a few large formulae for $\dfrac{\mathrm{d}^k}{\mathrm{d}x^k}P_\ell^m(x)$ in [38], some of which require hypergeometric series.

A Fortran program of (2.71) is created. A few sample calculations illustrating the method are included in Table 2.3. The results are compared to Maple 11's output with 18 correct digits in the evalf command.

x	ℓ	m	k	Formula (2.71)	Values$^{\text{evalf}[18]}$
0.5	1	1	1	.5773502691896257(0)	.5773502691896258(0)
0.0	2	1	5	.4500000000000000(2)	.4500000000000000(2)
0.5	2	1	5	.4105601914237338(3)	.4105601914237339(3)
0.0	7	5	8	.8431644375000000(9)	.8431644375000000(9)
0.5	7	5	8	.4152543313723771(10)	.4152543313723771(10)
0.5	15	7	11	.1849994958475265(21)	.1849994958475265(21)

Table 2.3: Numerical Evaluation of $\dfrac{\mathrm{d}^k}{\mathrm{d}x^k} P_\ell^m(x)$.

2.C.2 Chebyshev polynomials of the first kind

The Rodrigues formula for Chebyshev polynomials of the first kind is indeed very similar to that satisfied by Legendre functions [37]:

$$T_n(x) = \frac{\Gamma\left(\frac{1}{2}\right)}{(-2)^n \, \Gamma\left(n+\frac{1}{2}\right)} (1-x^2)^{\frac{1}{2}} \frac{\mathrm{d}^n}{\mathrm{d}x^n} (1-x^2)^{n-\frac{1}{2}}. \tag{2.74}$$

Therefore, it is natural with the help of the Leibniz Formula (Formula 2.0.1) to define the higher order derivatives of these functions as:

$$\frac{\mathrm{d}^i}{\mathrm{d}x^i} T_n(x) = \frac{\Gamma\left(\frac{1}{2}\right)}{(-2)^n \, \Gamma\left(n+\frac{1}{2}\right)} \sum_{l=0}^{i} \binom{i}{l} \frac{\mathrm{d}^l}{\mathrm{d}x^l} \left(1-x^2\right)^{\frac{1}{2}} \frac{\mathrm{d}^{n+i-l}}{\mathrm{d}x^{n+i-l}} \left(1-x^2\right)^{n-\frac{1}{2}}. \tag{2.75}$$

Without going into great detail, we regard this example as identical to the previous one. We apply the result of Corollary 2.1.1 and develop as the final result:

$$\frac{\mathrm{d}^k}{\mathrm{d}x^k}T_n(x) = \frac{\Gamma\left(\frac{1}{2}\right)}{(-2)^n\,\Gamma\left(n+\frac{1}{2}\right)}\sum_{l=0}^{k}\binom{k}{l}\left\{\left[\sum_{i=\lfloor\frac{l+1}{2}\rfloor}^{l}\hat{A}_l^i\,x^{2i-l}\,(-2)^i\,(1-x^2)^{\frac{1}{2}-i}\prod_{j=0}^{i-1}\left(\frac{1}{2}-j\right)\right]\right.$$
$$\left.\times\left[\sum_{i=\lfloor\frac{n+k-l+1}{2}\rfloor}^{n+k-l}\hat{A}_{n+k-l}^i\,x^{2i-n-k+l}\,(-2)^i\,(1-x^2)^{n-\frac{1}{2}-i}\prod_{j=0}^{i-1}\left(n-\frac{1}{2}-j\right)\right]\right\}. \tag{2.76}$$

with coefficients $\hat{A}_k^i$ given by (2.22).

A Fortran program of (2.76) is created. A few sample calculations illustrating the method are included in Table 2.4. The results are compared to Maple 11's output with 18 correct digits in the evalf command.

k	Formula (2.76)	Values$^{\text{evalf[18]}}$
1	-.743750000000000(1)	-.743750000000000(1)
2	.277500000000000(2)	.277500000000000(2)
3	.522000000000000(3)	.522000000000000(3)
4	-.108000000000000(4)	-.108000000000000(4)
5	-.326400000000000(5)	-.326400000000000(5)
6	-.230400000000000(5)	-.230400000000000(5)
7	.129024000000000(7)	.129024000000000(7)

Table 2.4: Numerical Evaluation of $\frac{\mathrm{d}^k}{\mathrm{d}x^k}T_n(x)$, with $(n,x) = (8, 0.25)$.

2.C.3 Hermite functions

Normalized Hermite functions are defined as [37]:

$$\psi_n(x) = \frac{e^{-x^2/2}}{\sqrt{n!\,2^n\,\sqrt{\pi}}}\,H_n(x), \tag{2.77}$$

where the Hermite polynomials $H_n(x)$ are defined as [37]:

$$H_n(x) = (-1)^n e^{x^2} \frac{\mathrm{d}^n}{\mathrm{d}x^n} e^{-x^2}. \tag{2.78}$$

Hermite polynomials satisfy the properties [37]:

$$\begin{cases} H_{n+1}(x) &= 2\,x\,H_n(x) - 2\,n\,H_{n-1}(x) \\ \dfrac{\mathrm{d}^i}{\mathrm{d}x^i} H_n(x) &= 2^i\,H_{n-i}(x) \displaystyle\prod_{j=0}^{i-1} (n-j), \end{cases} \tag{2.79}$$

where $H_l(x) \equiv 0$ for all $l < 0$. In addition, $e^{-x^2/2}$ satisfies:

$$\frac{\mathrm{d}^k}{\mathrm{d}x^k} e^{-x^2/2} = e^{-x^2/2} \sum_{i=\lfloor \frac{k+1}{2} \rfloor}^{k} (-1)^i \hat{A}_k^i\, x^{2i-k}, \tag{2.80}$$

with coefficients $\hat{A}_k^i$ given by (2.22).

Therefore, with the help of the Leibniz Formula (Formula 2.0.1) and equation (2.80), higher order derivatives of $\psi_n(x)$ are given by:

$$\frac{\mathrm{d}^k}{\mathrm{d}x^k} \psi_n(x) = \frac{e^{-x^2/2}}{\sqrt{n! 2^n \sqrt{\pi}}} \sum_{l=0}^{k} \binom{k}{l} \left[\sum_{i=\lfloor \frac{l+1}{2} \rfloor}^{l} (-1)^i\, \hat{A}_l^i\, x^{2i-l}\, 2^{k-l}\, H_{n-k+l}(x) \prod_{j=0}^{k-l-1} (n-j) \right]. \tag{2.81}$$

A Fortran program of (2.81) is created. A few sample calculations illustrating the method are included in Table 2.5. The results are compared to Maple 11's output with 18 correct digits in the evalf command.

2.C.4 Bessel functions

There are essentially eight different Bessel functions, that arise as the radial solutions to the Helmholtz equation $\nabla^2 u = -v^2 u$, in cylindrical or spherical

k	Formula (2.81)	Values[evalf[18]]
1	.129922131632585(1)	.129922131632585(1)
2	.183728266955170(0)	.183728266955170(0)
3	-.919953679539818(1)	-.919953679539817(1)
4	.905517887136197(1)	.905517887136197(1)
5	.743968246692044(2)	.743968246692044(2)
6	-.208374101622443(3)	-.208374101622443(3)
7	-.523664931165155(3)	-.523664931165155(3)

Table 2.5: Numerical Evaluation of $\frac{\mathrm{d}^k}{\mathrm{d}x^k}\psi_n(x)$, with $(n, x) = (5, 2)$.

coordinates:

$$x^2 f''(x) + x f'(x) + \left(v^2 x^2 - n^2\right) f(x) = 0 \qquad \text{in cylindrical coordinates,} \tag{2.82}$$

$$x^2 f''(x) + 2x f'(x) + \left(v^2 x^2 - n(n+1)\right) f(x) = 0 \qquad \text{in spherical coordinates.} \tag{2.83}$$

In the literature [37], the normal convention adopted for representing Bessel functions arising in cylindrical and spherical coordinates, is given by:

Kind	Cylindrical	Spherical
First	$J_n(v\,x)$	$j_n(v\,x)$
Second	$Y_n(v\,x)$	$y_n(v\,x)$
Modified First	$I_n(v\,x)$	$i_n(v\,x)$
Modified Second	$K_n(v\,x)$	$k_n(v\,x)$

The first column specifies the cylindrical Bessel functions, while the second column specifies the spherical Bessel functions. Each of the four Bessel functions arise from the same differential equation (2.82) or (2.83), depending on the allowed values of v, n and the function itself as its argument approaches the origin or tends to infinity. In addition, there is a general conversion between Bessel functions in cylindrical coordinates and Bessel functions in spherical coordinates such that:

$$c_n(v\,x) = \sqrt{\frac{\pi}{2\,v\,x}}\,C_{n+1/2}(v\,x), \tag{2.84}$$

where c represents any one of j, y, i, or k and where C represents the respective J, Y, I, or K. Bessel functions of the first kind arise when v and n are real. Bessel functions of the second kind are expressed as a combination of Bessel functions of the first kind in order to provide a second linearly independent solution to the second order differential equation. These functions only arise when the solution need not be defined at the origin, when v is real, and when n is an integer. Modified Bessel functions of the first kind, I, are intimately related to Bessel functions of the first kind, J. They arise when v is imaginary, and when n is real. These functions are finite at the origin, but tend to infinity as their arguments become large. Modified Bessel functions of the second kind are expressed as a combination of modified Bessel functions of the first kind in order to provide a second linearly independent solution to the differential equation. These functions only arise when the solution need not be defined at the origin, when v is imaginary, and when n is an integer. Employing the method of Frobenius [37] to solve (2.82), Bessel functions of the first kind are expressed as:

$$J_n(v\,x) = \sum_{k=0}^{\infty} \frac{(-1)^k}{k!\,\Gamma(k+n+1)} \left(\frac{v\,x}{2}\right)^{2k+n}, \tag{2.85}$$

although there are many more numerically stable formulae that exist. One remarkably numerically stable formulation, as developed in [39], expresses both the recurrence relation for Bessel functions of higher order and the infinite series as continued fractions. This method for the computation of continued fractions and simple forward recurrence can be combined to yield highly accurate evaluations of Bessel functions.

The general Bessel derivative recurrence relation, valid for $J_n(v\,x)$, $Y_n(v\,x)$, $K_n(v\,x)$, $j_n(v\,x)$, $y_n(v\,x)$ and $k_n(v\,x)$ is given by:

$$C_n'(v\,x) = \frac{n}{x}\,C_n(v\,x) - v\,C_{n+1}(v\,x). \tag{2.86}$$

This equation can be generalized as:

$$C_{n+k}(v\,x) = (-1)^k\,\frac{x^{n+k}}{v^k}\left(\frac{\mathrm{d}}{x\mathrm{d}x}\right)^k (x^{-n}\,C_n(v\,x)). \tag{2.87}$$

We are now ready to apply Theorem 2.1 with $(\mu,\nu,m,n) = (0,0,1,n)$ to obtain:

$$\frac{\mathrm{d}^k}{\mathrm{d}x^k}C_n(v\,x) = \sum_{i=0}^{k}(-1)^i\,\frac{v^i\,C_{n+i}(v\,x)}{x^{k-i}}\,A_k^i, \tag{2.88}$$

with coefficients A_k^i given by (2.7).

The Bessel derivative recurrence relation valid for $I_n(v\,x)$ and $i_n(v\,x)$:

$$\widetilde{C}_n'(v\,x) = \frac{n}{x}\,\widetilde{C}_n(v\,x) + v\,\widetilde{C}_{n+1}(v\,x), \tag{2.89}$$

gives a similar result:

$$\widetilde{C}_{n+k}(v\,x) = \frac{x^{n+k}}{v^k}\left(\frac{\mathrm{d}}{x\mathrm{d}x}\right)^k (x^{-n}\,\widetilde{C}_n(v\,x)), \tag{2.90}$$

which, after application of Theorem 2.1 with $(\mu,\nu,m,n) = (0,0,1,n)$, yields:

$$\frac{\mathrm{d}^k}{\mathrm{d}x^k}\widetilde{C}_n(v\,x) = \sum_{i=0}^{k}\frac{v^i\,\widetilde{C}_{n+i}(v\,x)}{x^{k-i}}\,A_k^i, \tag{2.91}$$

with the same coefficients A_k^i. A few sample calculations illustrating the method applied to $j_n(v\,x)$, $I_n(v\,x)$, $k_n(v\,x)$ and $Y_n(v\,x)$ are included in Tables 2.6–2.9. The computation of the Bessel functions is performed using the programs presented in [40]. The results are compared to Maple 11's output with different values of correct digits in the evalf command. In Tables 2.6–2.9, the first four columns are relative errors, evaluated to 15 digits, between the method and Maple 11's evalf[64], while the last column is the value of evalf[64] to 15 digits.

In the literature [41], a formula exists expressing the higher order derivatives of Bessel functions as a sum of the Bessel functions and their first derivatives; it requires recurrence relations to solve for the coefficients of the Bessel functions and their first derivatives. However, a differentiation of the previous coefficient is performed in these recurrence relations, which limits the formula's practicality. In contrast, the recurrence relations we obtain for the coefficients A_k^i pose no computational problems. Also in the literature [42], there exist a few other formulae for higher order derivatives of Bessel functions. None of these is, however, as concise or as general as (2.88) and (2.91). In addition, these formulae often require evaluation of hypergeometric series, while our formulae do not.

2.C.5 Treatment of differential equations

Theorem 2.2: *For a function $f(x)$ satisfying an m^{th} order linear homogeneous differential equation of the form:*

$$f(x) = \sum_{k=1}^{m} p_k(x)\,\frac{\mathrm{d}^k}{\mathrm{d}x^k} f(x), \tag{2.92}$$

k	Formula (2.88)$^{(\dagger)}$	evalf[15]$^{(\dagger)}$	evalf[22]$^{(\dagger)}$	evalf[28]$^{(\dagger)}$	Values$^{\text{evalf[64]}}$
11	.000(0)	.119(-4)	.639(-12)	.000(0)	-.459687936963032(-1)
12	.000(0)	.124(-3)	.632(-11)	.000(0)	.572920121838019(-1)
13	.000(0)	.255(-2)	.140(-9)	.000(0)	.393828142346694(-1)
14	.000(0)	.310(-1)	.184(-8)	.000(0)	-.504399076519013(-1)
15	.000(0)	.715(0)	.348(-7)	.871(-14)	-.344324623774753(-1)

$^{(\dagger)}$ Relative Error of given formula with respect to Values$^{\text{evalf[64]}}$.

Table 2.6: Numerical Evaluation of $\dfrac{\mathrm{d}^k}{\mathrm{d}x^k} j_n(v\,x)$, with $(n, v, x) = (1, 1, 1)$.

k	Formula (2.91)$^{(\dagger)}$	evalf[15]$^{(\dagger)}$	evalf[22]$^{(\dagger)}$	evalf[28]$^{(\dagger)}$	Values$^{\text{evalf[64]}}$
11	.000(0)	.175(-7)	.295(-14)	.000(0)	.338766805941983(0)
12	.000(0)	.105(-6)	.779(-13)	.000(0)	.243783774241269(0)
13	.000(0)	.265(-5)	.633(-12)	.000(0)	.315639838946200(0)
14	.000(0)	.677(-4)	.985(-11)	.000(0)	.228794506240254(0)
15	.000(0)	.102(-2)	.679(-10)	.000(0)	.296695084720158(0)

$^{(\dagger)}$ Relative Error of given formula with respect to Values$^{\text{evalf[64]}}$.

Table 2.7: Numerical Evaluation of $\dfrac{\mathrm{d}^k}{\mathrm{d}x^k} I_n(v\,x)$, with $(n, v, x) = (1, 1, 1)$.

the function $f(x^{\mu+1})$, $\mu \in \mathbb{R}$ satisfies the following differential equation:

$$f(x^{\mu+1}) = \sum_{i=1}^{m} \bar{p}_i(x)\, \frac{\mathrm{d}^i}{\mathrm{d}x^i} f(x^{\mu+1}), \tag{2.93}$$

where:

$$\bar{p}_i(x) = \sum_{k=i}^{m} \frac{p_k(x^{\mu+1})}{(\mu+1)^k}\, x^{i-k(\mu+1)} \sum_{j=0}^{i} \frac{(-1)^{i-j}\,(j-(k-1)(\mu+1))_{k,\mu+1}}{j!\,(i-j)!}. \tag{2.94}$$

Proof. By making the substitution $x \leftrightarrow x^{\mu+1}$ in the differential equation (2.92),

k	Formula (2.88)$^{(\dagger)}$	evalf[15]$^{(\dagger)}$	evalf[22]$^{(\dagger)}$	evalf[28]$^{(\dagger)}$	Values$^{\text{evalf[64]}}$
11	.188(-12)	.265(-14)	.000(0)	.000(0)	-.752413953761027(09)
12	.450(-12)	.204(-14)	.000(0)	.000(0)	.978138139947121(10)
13	.876(-13)	.000(0)	.000(0)	.000(0)	-.136939339593175(12)
14	.301(-11)	.000(0)	.000(0)	.000(0)	.205409009389820(13)
15	.280(-11)	.304(-14)	.000(0)	.000(0)	-.328654415023718(14)

$^{(\dagger)}$ Relative Error of given formula with respect to Values$^{\text{evalf[64]}}$.

Table 2.8: Numerical Evaluation of $\dfrac{\mathrm{d}^k}{\mathrm{d}x^k} k_n(v\,x)$, with $(n, v, x) = (1, 1, 1)$.

k	Formula (2.88)$^{(\dagger)}$	evalf[15]$^{(\dagger)}$	evalf[22]$^{(\dagger)}$	evalf[28]$^{(\dagger)}$	Values$^{\text{evalf[64]}}$
11	.600(-12)	.000(0)	.000(0)	.000(0)	.252974959307709(8)
12	.559(-12)	.329(-14)	.000(0)	.000(0)	-.303796293136156(9)
13	.427(-11)	.253(-14)	.000(0)	.000(0)	.395162430091925(10)
14	.376(-11)	.361(-14)	.000(0)	.000(0)	-.553478113668334(11)
15	.784(-11)	.240(-14)	.000(0)	.000(0)	.830518694305487(12)

$^{(\dagger)}$ Relative Error of given formula with respect to Values$^{\text{evalf[64]}}$.

Table 2.9: Numerical Evaluation of $\dfrac{\mathrm{d}^k}{\mathrm{d}x^k} Y_n(v\,x)$, with $(n, v, x) = (1, 1, 1)$.

we obtain:

$$\begin{aligned} f(x^{\mu+1}) &= \sum_{k=1}^{m} p_k(x^{\mu+1}) \, \frac{\mathrm{d}^k}{\mathrm{d}(x^{\mu+1})^k} f(x^{\mu+1}) \\ &= \sum_{k=1}^{m} \frac{p_k(x^{\mu+1})}{(\mu+1)^k} \left(\frac{\mathrm{d}}{x^{\mu}\mathrm{d}x} \right)^k f(x^{\mu+1}) \\ &= \sum_{k=1}^{m} \frac{p_k(x^{\mu+1})}{(\mu+1)^k} \sum_{i=1}^{k} A_k^i \, x^{i-k(\mu+1)} \, \frac{\mathrm{d}^i}{\mathrm{d}x^i} f(x^{\mu+1}), \end{aligned} \tag{2.95}$$

where we have employed Theorem 2.1 with $(\mu, \nu, m, n) = (\mu, 0, 0, 0)$ in the last step, and where it is important to note that $A_k^0 = 0$ for $k > 0$ for this specific case.

By reversing the order of summation, we have:

$$f(x^{\mu+1}) = \sum_{i=1}^{m} \frac{\mathrm{d}^i}{\mathrm{d}x^i} f(x^{\mu+1}) \sum_{k=i}^{m} \frac{p_k(x^{\mu+1})}{(\mu+1)^k}\, x^{i-k(\mu+1)}\, A_k^i,$$

and we obtain (2.93) and (2.94) by replacing coefficients A_k^i by their analytical expression (2.8) and by defining $\bar{p}_i(x)$ as the summation over k. □

Remark: The asymptotic behaviour of the functions $\bar{p}_i(x)$ as $x \to \infty$ remains invariant under the substitution $x^{\mu+1} \leftrightarrow x^{\mu+1}\left(a_0 + \frac{a_1}{x} + \cdots +\right)$.

As an example of application of Theorem 2.2, we solve the second order linear differential equation:

$$f(x) = \left(\frac{1}{9x^5} - \frac{1}{3x^2}\right) \frac{\mathrm{d}}{\mathrm{d}x} f(x) - \frac{1}{18x^4} \frac{\mathrm{d}^2}{\mathrm{d}x^2} f(x), \tag{2.96}$$

where:

$$p_1(x) = \frac{1}{9x^5} - \frac{1}{3x^2} \quad \text{and} \quad p_2(x) = -\frac{1}{18x^4}.$$

After the substitution $x \leftrightarrow x^{\mu+1}$, we find:

$$\bar{p}_1(x) = \frac{1}{9(\mu+1)\, x^{6\mu+5}} - \frac{1}{3(\mu+1)\, x^{3\mu+2}} + \frac{\mu}{18(\mu+1)^2\, x^{6\mu+5}} \tag{2.97}$$

$$\bar{p}_2(x) = \frac{-1}{18(\mu+1)^2\, x^{6\mu+4}}, \tag{2.98}$$

which, after wisely choosing $\mu = -\frac{2}{3}$, simplifies the equation to:

$$f(x^{\frac{1}{3}}) = -\frac{\mathrm{d}}{\mathrm{d}x} f(x^{\frac{1}{3}}) - \frac{1}{2} \frac{\mathrm{d}^2}{\mathrm{d}x^2} f(x^{\frac{1}{3}}), \tag{2.99}$$

admitting the solution $f(x^{\frac{1}{3}}) = e^{-x}(a \sin(x) + b \cos(x))$.

Ultimately, the solution of our initial differential equation is then:

$$f(x) = e^{-x^3}\left(a\sin(x^3) + b\cos(x^3)\right), \tag{2.100}$$

which would not have been trivial to solve using a power series expansion or Laplace transform.

This example serves to illustrate the capabilities of Theorem 2.2, the substitution $x \leftrightarrow x^{\mu+1}$ allows one to attempt to match the (linear homogeneous) differential equation at hand with any differential equation that has been studied in depth, not only a simple one where the coefficients $\bar{p}_i(x)$ are constant.

Analytical remainder estimate from a differential equation

Extrapolation methods requiring an analytical remainder estimate of the integrand are among the most accurate and fast methods developed for evaluating molecular integrals formulated as spherical Bessel integral functions [14–19]. As part of the envelope of the spherical Bessel integral functions, reduced Bessel functions $\hat{k}_{n-\frac{1}{2}}(x)$ are defined as [43]:

$$\hat{k}_{n-\frac{1}{2}}(x) = \sqrt{\frac{2}{\pi}}x^{n-\frac{1}{2}}K_{n-\frac{1}{2}}(x) = \sum_{j=1}^{n}\frac{(2n-j-1)!}{(j-1)!(n-j)!}\frac{x^{j-1}e^{-x}}{2^{n-1}}, \tag{2.101}$$

and satisfy the differential equation:

$$\hat{k}_{n-\frac{1}{2}}(x) = -\frac{2(n-1)}{x}\frac{\mathrm{d}}{\mathrm{d}x}\hat{k}_{n-\frac{1}{2}}(x) + \frac{\mathrm{d}^2}{\mathrm{d}x^2}\hat{k}_{n-\frac{1}{2}}(x). \tag{2.102}$$

Considering that their argument in the spherical Bessel integral functions is $\gamma(x) = \sqrt{\tau + \kappa x^2}$ and noting that $\gamma(x)$ has the asymptotic expansion as

$x \to \infty$:

$$\gamma(x) = \sum_{n=0}^{\infty} \binom{1/2}{n} \frac{\tau^n}{\kappa^{n-\frac{1}{2}}\, x^{2n-1}} = x\,\sqrt{\kappa}\left(1 + \frac{\tau}{2\kappa\, x^2} - \frac{\tau^2}{8\kappa^2\, x^4} + \cdots +\right), \tag{2.103}$$

the asymptotic behaviour of the coefficients in (2.102) remains unchanged for the composition $\hat{k}_{n-\frac{1}{2}}[\gamma(x)]$. Notably, $\bar{p}_1(x) \sim x^{-1}$ and $\bar{p}_2(x) \sim 1$ as $x \to \infty$ (For $n = 1$, $\bar{p}_1(x) \sim 1$ and $\bar{p}_2(x) = 0$ as $x \to \infty$). This result follows naturally from the development of Theorem 2.2 and the subsequent remark, but would have been difficult to obtain by hand.

2.D Numerical discussion

The implications of Theorem 2.1 are twofold. Analytically speaking, compact formulae of higher order derivatives of some special functions are producible; numerically speaking, these formulae are *critical.* The straightforward calculation of $\left.\frac{\mathrm{d}^{14}}{\mathrm{d}x^{14}} j_n(v\,x)\right|_{(n,v,x)=(1,1,1)}$ using Maple 11's evalf command to 15 correct digits yields -0.052008. The number is only accurate to one digit, the true value being -0.050439 90765 19013. In this case, an accuracy of 28 digits in Maple 11's evalf command is required. A double precision Fortran code of (2.88) or (2.91) gives an evaluation to 15 correct digits instantly. This problem in accuracy and calculation time worsens when even higher order derivatives are needed.

Referring to Tables 2.3–2.9, Theorem 2.1 is accurate to 15 correct digits evaluated in double precision. This implementation in Fortran is remarkable because all of the examples of Theorem 2.1 draw from the same coefficients A_k^i, and all have the same $(k+1)$-term summation. This is very practical from a computational perspective. With the recursive representation of the coefficients, to calculate a certain derivative, only the coefficients of lower order derivatives are required and not the lower order derivatives themselves. This makes each derivative more independent from lower order derivatives. In contrast, a recursive algorithm, like one stemming from a differential equation, may diverge quite quickly.

Although Tables 2.6 and 2.7 highlight the efficacy of (2.88) and (2.91), Tables 2.8 and 2.9 show their limitations, especially concerning the evaluation of the derivatives of $k_n(v\,x)$ and $Y_n(v\,x)$. Formula (2.88) does not achieve complete machine precision for these functions because for $(v, x) = (1, 1)$, (2.88) becomes an alternating series with each term approximately one order of magnitude larger than the previous term. In this context, the summation is susceptible to round-off error. This does not occur when computing the derivatives of $j_n(v\,x)$ because each term is not significantly larger or smaller than the previous one. This also does not occur when computing the derivatives of $I_n(v\,x)$, as (2.91) is not an alternating series. Interestingly, Maple 11 seems to show no difficulty computing the derivatives of $k_n(v\,x)$ or $Y_n(v\,x)$, the modified Bessel functions.

In Tables 2.3, 2.4 and 2.5, we list the values obtained using the formulae (2.71), (2.76) and (2.81) respectively. In these tables, values with 18 correct digits are obtained using Maple 11 evalf[18] and they are referred to as $\text{Values}^{\text{evalf}[18]}$. In Tables 2.6, 2.7, 2.8 and 2.9, we list the relative errors with respect to values obtained using Maple 11 evalf[64], which are referred to as $\text{Values}^{\text{evalf}[64]}$. In these tables, we list the relative errors obtained using our formulae, Maple's evalf[15], evalf[22] and evalf[28].

In all tables, the numbers in parentheses represent powers of 10.

Chapter 3

The $G_n^{(m)}$ Transformation

3.A Definitions and basic properties

Let the natural numbers be denoted by $\mathbb{N} = \{1, 2, 3, \ldots\}$, and $\mathbb{N}_0 = \{0, 1, 2, 3, \ldots\}$. The integers are $\mathbb{Z} = \{\ldots -3, -2, -1, 0, 1, 2, 3, \ldots\}$, and let $\mathbb{Q}, \mathbb{R}, \mathbb{C}$ denote the rational, real, and complex numbers, respectively.

Let f and g be functions defined on $D \subset X \to Y$, where the sets X and Y could represent either the real numbers $\mathbb{R}$ or the complex numbers $\mathbb{C}$. Let A be a subset of D. Let X_∞ be one of the sets $\mathbb{R}_\infty = \mathbb{R} \cup \{-\infty, \infty\}$ or $\mathbb{C}_\infty = \mathbb{C} \cup \{\infty\}$. Suppose $z_0 \in \overline{A} \subset X_\infty$ (i.e. z_0 is a limit point of A).

Definition ([5]): We say f is in the order of g as $z \to z_0$ on $A \subset X_\infty$ if X_∞ contains a neighbourhood U of z_0 such that for some M:

$$z \in U \cap A \Longrightarrow |f(z)| \leq M|g(z)|. \tag{3.1}$$

We write $f(z) = \mathcal{O}(g(z))$ as $z \to z_0$. Equivalently, if g is nonzero near

$z_0 \in \bar{A}$, then:

$$\limsup_{\substack{z \to z_0 \\ z \in A}} \left| \frac{f(z)}{g(z)} \right| < \infty, \tag{3.2}$$

or $\left|\dfrac{f}{g}\right|$ is bounded on A near z_0.

Definition ([5]): We say f is in the little order of g as $z \to z_0$ on $A \subset X_\infty$ if for all $\epsilon > 0$, X_∞ contains a neighbourhood U_ϵ of z_0 such that:

$$z \in U_\epsilon \cap A \Longrightarrow |f(z)| \leq \epsilon |g(z)|. \tag{3.3}$$

We write $f(z) = o(g(z))$ as $z \to z_0$. Equivalently, if g is nonzero near $z_0 \in \bar{A}$ and $f(z_0) = 0$ when $z_0 \in A$, then:

$$\lim_{\substack{z \to z_0 \\ z \in A}} \frac{f(z)}{g(z)} = 0. \tag{3.4}$$

Definition ([5]): If $f - g = o(g)$ $(z \to z_0 \in A)$, we say f is asymptotic to g as $z \to z_0$ on $A \subset X_\infty$ and write $f(z) \sim g(z)$ as $z \to z_0$. Equivalently, if g is nonzero near $z_0 \in \bar{A}$ and $f(z_0) = g(z_0)$ when $z_0 \in A$, then $f \sim g$ is equivalent to:

$$\lim_{\substack{z \to z_0 \\ z \in A}} \frac{f(z)}{g(z)} = 1. \tag{3.5}$$

We define the class of functions we denote $\mathbf{A}^{(\gamma)}$ by

Definition ([5, 12]): A function $\alpha(x)$ defined for all large $x > 0$ is in the set $\mathbf{A}^{(\gamma)}$ if it has a Poincaré-type asymptotic expansion of the form:

$$\alpha(x) \sim \sum_{i=0}^{\infty} \alpha_i x^{\gamma - i}, \qquad x \to +\infty. \tag{3.6}$$

If, in addition, $\alpha_0 \neq 0$ in (3.6), then $\alpha(x)$ is said to belong to $\mathbf{A}^{(\gamma)}$ strictly. Here γ is complex in general.

Building on this class of functions, we also have the

Definition ([5, 12]): A function $f(x)$ belongs to the set $\mathbf{B}^{(m)}$ if it satisfies a linear homogeneous differential equation of order m of the form:

$$f(x) = \sum_{k=1}^{m} p_k(x) f^{(k)}(x), \tag{3.7}$$

where $p_k \in \mathbf{A}^{(k)}$, $k = 1, \ldots, m$, such that $p_k \in \mathbf{A}^{(i_k)}$ strictly for some integer $i_k \leq k$.

3.B The $G_n^{(m)}$ transformation

Let $F(x) = \int_0^x f(t)\,\mathrm{d}t$ and let $I[f] = \lim_{x\to\infty} F(x)$. Now, for functions in $\mathbf{B}^{(m)}$, we can construct the asymptotic remainder of the difference between $F(x)$ and $I[f]$. We have the

Theorem 3.1 ([12]): *Let $f(x) \in \mathbf{B}^{(m)}$ and let $f(x)$ be integrable on $[0, \infty)$ (i.e. $\int_0^\infty f(t)\,\mathrm{d}t < \infty$). If for $1 \leq i \leq m$ and $i \leq k \leq m$, we have $\lim_{x\to\infty} p_k^{(i-1)}(x)\, f^{(k-i)}(x) = 0$ and for every integer $l \geq -1$, we have $\sum_{k=1}^{m} l(l-1)\cdots(l-k+1)p_{k,0} \neq 1$ where $p_{k,0} = \lim_{x\to\infty} x^{-k}\, p_k(x)$ for $1 \leq k \leq m$, then as $x \to \infty$, we have:*

$$I[f] - F(x) = \int_x^\infty f(t)\,\mathrm{d}t \sim \sum_{k=0}^{m-1} x^{\sigma_k}\, f^{(k)}(x) \left(\beta_{0,k} + \frac{\beta_{1,k}}{x} + \frac{\beta_{2,k}}{x^2} + \cdots + \right), \tag{3.8}$$

for some integers $\sigma_k \leq k+1$ for $k = 0, \ldots, m-1$.

To solve for the unknowns $\beta_{k,i}$, we must set up and solve a system of linear equations. To produce this system of linear equations, few methods have been conceived. The first is called the $D_n^{(m)}$ transformation. For this transformation, a set of interpolating points $x_0, x_1, \ldots, x_l$ is used to solve for the unknowns. If we take the limiting case as all the points coalesce, we achieve the first confluent form [5] of the $D_n^{(m)}$ transformation, known as the $G_n^{(m)}$ transformation [13]. The approximation $G_n^{(m)}$ to $\int_0^\infty f(t)\mathrm{d}t$ is given as the solution of the system of $mn+1$ linear equations [13]:

$$\frac{\mathrm{d}^l}{\mathrm{d}x^l}\left\{G_n^{(m)} - \int_0^x f(t)\,\mathrm{d}t - \sum_{k=0}^{m-1} x^{\sigma_k} f^{(k)}(x) \sum_{i=0}^{n-1} \frac{\bar{\beta}_{k,i}}{x^i}\right\} = 0, \quad l = 0, 1, \ldots, mn, \tag{3.9}$$

where it is assumed that $\frac{\mathrm{d}^l}{\mathrm{d}x^l} G_n^{(m)} \equiv 0, \forall l > 0$. In the above system (3.9), $\sigma_k = \min(s_k, k+1)$ where s_k is the largest of the integers s such that $\lim_{x\to\infty} x^s f^{(k)}(x) = 0$ holds, $k = 0, 1, \ldots, m-1$. Also, $G_n^{(m)}$ and $\bar{\beta}_{k,i}$ are the respective set of $mn+1$ unknowns.

3.C An algorithm for the $G_n^{(1)}$ transformation

The $G_n^{(1)}$ transformation can be written as the solution to the linear system (3.9) with $m = 1$.

Instead of solving the system of linear equations each time for each order n, it would be ideal to resolve each approximation $G_n^{(1)}$ in a recursive manner.

By considering the equation for $l = 0$:

$$G_n^{(1)} - F(x) = x^{\sigma_0} f(x) \sum_{i=0}^{n-1} \frac{\bar{\beta}_{0,i}}{x^i} \quad \text{with} \quad F(x) = \int_0^x f(t)\mathrm{d}t, \tag{3.10}$$

and by isolating the summation on the right hand side, we obtain:

$$\frac{G_n^{(1)} - F(x)}{x^{\sigma_0} f(x)} = \sum_{i=0}^{n-1} \frac{\bar{\beta}_{0,i}}{x^i}. \tag{3.11}$$

To eliminate the summation, and consequently all of the unknowns $\bar{\beta}_{0,i}$, we must apply some type of operator to both sides of the equation. In the non-confluent case, this is achieved by the divided difference operator acting on the different interpolation points of the $D_n^{(1)}$ transformation. This culminates with the conception of the W algorithm [5]. In the confluent case, we require the $\left(x^2 \frac{\mathrm{d}}{\mathrm{d}x}\right)$ operator, which, applied n times, eliminates the summation. For example, if we apply the $\left(x^2 \frac{\mathrm{d}}{\mathrm{d}x}\right)$ operator to the summation, we obtain:

$$\left(x^2 \frac{\mathrm{d}}{\mathrm{d}x}\right) \left(\sum_{i=0}^{n-1} \frac{\bar{\beta}_{0,i}}{x^i}\right) = x^2 \sum_{i=1}^{n-1} \frac{-i\,\bar{\beta}_{0,i}}{x^{i+1}} = \sum_{i=1}^{n-1} \frac{-i\,\bar{\beta}_{0,i}}{x^{i-1}} \tag{3.12}$$

and the first unknown $\bar{\beta}_{0,0}$ disappears. Successive application will continue to eliminate the unknowns in this fashion and we obtain:

$$\left(x^2 \frac{\mathrm{d}}{\mathrm{d}x}\right)^n \left[\frac{G_n^{(1)} - F(x)}{x^{\sigma_0} f(x)}\right] = 0 \quad \Longrightarrow \quad G_n^{(1)} = \frac{\left(x^2 \frac{\mathrm{d}}{\mathrm{d}x}\right)^n \left(\frac{F(x)}{x^{\sigma_0} f(x)}\right)}{\left(x^2 \frac{\mathrm{d}}{\mathrm{d}x}\right)^n \left(\frac{1}{x^{\sigma_0} f(x)}\right)}, \tag{3.13}$$

which leads to a recursive algorithm for the $G_n^{(1)}$ transformation.

Algorithm 3.1.1:

1. Set:

$$\mathcal{N}_0(x) = \frac{F(x)}{x^{\sigma_0} f(x)} \qquad \text{and} \qquad \mathcal{D}_0(x) = \frac{1}{x^{\sigma_0} f(x)}. \tag{3.14}$$

2. For $n = 1, 2, \ldots$, compute $\mathcal{N}_n(x)$ and $\mathcal{D}_n(x)$ recursively from:

$$\mathcal{N}_n(x) = \left(x^2 \frac{\mathrm{d}}{\mathrm{d}x}\right) \mathcal{N}_{n-1}(x) \qquad \text{and} \qquad \mathcal{D}_n(x) = \left(x^2 \frac{\mathrm{d}}{\mathrm{d}x}\right) \mathcal{D}_{n-1}(x). \tag{3.15}$$

3. For all n, the approximations $G_n^{(1)}(x)$ to $\left(\int_0^x + \int_x^\infty\right) f(t)\,\mathrm{d}t$ are given by:

$$G_n^{(1)}(x) = \frac{\mathcal{N}_n(x)}{\mathcal{D}_n(x)}. \tag{3.16}$$

Since we are investigating integral tails $\int_x^\infty f(t)\,\mathrm{d}t$ rather than complete semi-infinite integrals, the remaining integrals $\int_0^x f(t)\,\mathrm{d}t$ appear on both sides of the above equation and we can then extract the approximation $\tilde{G}_n^{(1)}(x)$ to integral tails as follows:

$$\begin{aligned} \tilde{G}_n^{(1)}(x) &= G_n^{(1)}(x) - F(x) \\ &= \frac{\mathcal{N}_n(x) - F(x)\,\mathcal{D}_n(x)}{\mathcal{D}_n(x)} \\ &= \frac{\sum_{r=1}^{n} \binom{n}{r} \mathcal{D}_{n-r}(x) \, \left(x^2 \frac{\mathrm{d}}{\mathrm{d}x}\right)^{r-1} (x^2 f(x))}{\mathcal{D}_n(x)} \\ &= \frac{\tilde{\mathcal{N}}_n(x)}{\mathcal{D}_n(x)}. \end{aligned} \tag{3.17}$$

The development of an algorithm for the case of $m = 2$ (i.e. for the $G_n^{(2)}$ transformation) is of interest as many oscillatory integrals satisfy second order linear homogeneous differential equations of the form required for Theorem 3.1. For the case of $m > 1$, general algorithms could be constructed based on the E algorithm [2] and the FS algorithm [5]. However, as the G transformation is a confluent transformation, in that the linear system (3.9) is essentially created by differentiation, algorithms stemming from the E algorithm or the

FS algorithm would be symbolic in nature and perhaps inefficient, due to the recursive differentiation involved.

Chapter 4

The $G_n^{(1)}$ Transformation For Incomplete Bessel Functions and Tail Integrals of Probability Distributions

We use the algorithm for the $G_n^{(1)}$ transformation to approximate incomplete Bessel functions and tail probabilities of the normal distribution, the gamma distribution, the student's t-distribution, the inverse Gaussian distribution and Fisher's F distribution. Using this algorithm, which can be computed recursively when using symbolic programming languages, we are able to compute these integrals to high pre-determined accuracies. Previous to this contribution, the evaluation of these tail probabilities using the $G_n^{(1)}$ transformation required symbolic computation of large determinants and/or systems of linear equations. With the use of our algorithm, the $G_n^{(1)}$ transformation can be performed relatively easily to produce explicit approximations.

4.A Incomplete Bessel functions

Incomplete Bessel functions were a subject of significant research and we refer the interested reader to these articles [44–53] for a rich history of these functions. Of the many applications of incomplete Bessel functions, we note that they appear when Ewald-type summation acceleration procedures [54] are applied to electronic-structure calculations for systems described in terms of Gaussian-type atomic orbitals, with periodicity in one, two, or all three physical dimensions. Incomplete Bessel functions of zero order are also involved in numerous applications to electromagnetic waves [55–59].

4.A.1 Definitions and basic properties

Due to their integral representation [52]:

$$K_\nu(x,y) = \int_1^\infty \frac{e^{-x\,t-y/t}}{t^{\nu+1}}\,\mathrm{d}t, \tag{4.1}$$

incomplete Bessel functions are a computational challenge. Equipped with the developed algorithm, we apply the $G_n^{(1)}$ transformation to compute incomplete Bessel functions to high pre-determined accuracies. We also demonstrate that this algorithm allows for a broad range of incomplete Bessel computation.

Integration by parts of the integral representation of $K_\nu(x,y)$ in (4.1) leads to the inhomogeneous recurrence formula [60, 61]:

$$x\,K_{\nu-1}(x,y) + \nu\,K_\nu(x,y) - y\,K_{\nu+1}(x,y) = e^{-x-y}. \tag{4.2}$$

Defining the modified Bessel function using the formula [62]:

$$K_\nu(z) = \frac{1}{2}\int_0^\infty \frac{e^{-(z/2)(t+1/t)}}{t^{\nu+1}}\,\mathrm{d}t, \tag{4.3}$$

and defining $u = \sqrt{x\,y}$ and $v = \sqrt{\frac{x}{y}}$, we have another important functional relation [52]:

$$K_\nu(x,y) + K_{-\nu}(y,x) = 2\,v^\nu\,K_\nu(2\,u). \tag{4.4}$$

By interchanging $x \leftrightarrow y$, equation (4.4) can effectively double the applicable region of any algorithm, provided modified Bessel functions can be calculated. In terms of u and v, equation (4.1) can be expressed as [52]:

$$K_\nu(u,v) = \int_v^\infty \frac{v^\nu\,e^{-u(t+1/t)}}{t^{\nu+1}}\,\mathrm{d}t, \tag{4.5}$$

or, it can be expressed as a generalized incomplete gamma function [61, 63]:

$$K_\nu(x,y) = x^\nu\,\Gamma(-\nu;x;x\,y) \qquad \text{where} \qquad \Gamma(\alpha;x;b) = \int_x^\infty t^{\alpha-1}\,e^{-t-b/t}\,\mathrm{d}t. \tag{4.6}$$

4.A.2 Computing incomplete Bessel functions

Since incomplete Bessel functions satisfy a first order linear homogeneous differential equation, we use the $G_n^{(1)}$ transformation in order to obtain the evaluation of $K_\nu(x,y)$ for a wide range of the involved parameter and variables to a high pre-determined accuracy. We begin our numerical discussion with the following equation obtained from (4.6):

$$K_\nu(x,y) + x^\nu \int_0^x \frac{e^{-t-xy/t}}{t^{\nu+1}}\,\mathrm{d}t = x^\nu \int_0^\infty \frac{e^{-t-xy/t}}{t^{\nu+1}}\,\mathrm{d}t. \tag{4.7}$$

The integrand $f(t) = \dfrac{e^{-t-xy/t}}{t^{\nu+1}}$ in (4.7) satisfy the first order linear homogeneous differential equation given by:

$$f(t) = -\frac{t^2}{t^2 - x\,y + (\nu+1)\,t} f'(t), \tag{4.8}$$

whereupon we find that $f(t) \in \mathbf{B}^{(1)}$ and $\sigma_0 = 0$.

Symbolically programming the $G_1^{(1)}$ transformation to the right hand side of (4.7) through our algorithm gives:

$$\begin{aligned} G_1^{(1)}(x,y,\nu) &= \frac{\mathcal{N}_1(x)}{\mathcal{D}_1(x)} \\ &= \frac{x^{\nu+2}}{x^2 - x\,y + (\nu+1)\,x} f(x) + x^\nu \int_0^x \frac{e^{-t-xy/t}}{t^{\nu+1}} \mathrm{d}t. \end{aligned} \tag{4.9}$$

Since incomplete Bessel functions are defined as integral tails rather than complete semi-infinite integrals, the remaining integral appears on both sides of the equation. We can then extract the approximation to the functions $K_\nu(x,y)$, which is given by:

$$\tilde{G}_1^{(1)}(x,y,\nu) = \frac{x\,e^{-x-y}}{x^2 - x\,y + (\nu+1)\,x}. \tag{4.10}$$

Low order transformations like (4.10), however, may not be sufficient to cover the entire relevant range of the parameter ν and the variables x and y. By expanding the derivations involved in the functions $\mathcal{N}_n(x)$ and $\mathcal{D}_n(x)$ given by equation (3.16) in the algorithm, and by proceeding as above, we are able to develop explicitly the numerator $\tilde{\mathcal{N}}_n(x,y,\nu)$ and denominator $\mathcal{D}_n(x,y,\nu)$ of the approximations $\tilde{G}_n^{(1)}(x,y,\nu)$ for incomplete Bessel functions. The numerator

$\tilde{\mathcal{N}}_n(x,y,\nu)$ is given by:

$$\tilde{\mathcal{N}}_n(x,y,\nu) = \left(x^2\frac{\mathrm{d}}{\mathrm{d}x}\right)^n \left(\frac{F(x)}{x^{\sigma_0} f(x)}\right) - F(x)\left(x^2\frac{\mathrm{d}}{\mathrm{d}x}\right)^n \left(\frac{1}{x^{\sigma_0} f(x)}\right). \quad (4.11)$$

For the development of $\mathcal{D}_n(x,y,\nu)$, we use the Leibniz product rule and the SSF I with $(\mu,\nu,m,n) = (-2,-\nu-1,0,0)$ as follows:

$$\begin{aligned}
\mathcal{D}_n(x,y,\nu) &= \left(t^2\frac{\mathrm{d}}{\mathrm{d}t}\right)^n \left(t^{\nu+1}e^{t+xy/t}\right)\Big|_{t=x} \\
&= \sum_{r=0}^{n}\binom{n}{r}\left(t^2\frac{\mathrm{d}}{\mathrm{d}t}\right)^{n-r} e^{xy/t}\Big|_{t=x}\left(t^2\frac{\mathrm{d}}{\mathrm{d}t}\right)^{r}\left(t^{\nu+1}e^{t}\right)\Big|_{t=x} \\
&= \sum_{r=0}^{n}\binom{n}{r}(-x\,y)^{n-r}e^{y}\left(t^2\frac{\mathrm{d}}{\mathrm{d}t}\right)^{r}\left(t^{\nu+1}e^{t}\right)\Big|_{t=x} \\
&= \sum_{r=0}^{n}\binom{n}{r}(-x\,y)^{n-r}e^{y}\sum_{i=0}^{r}A_r^i\,t^{\nu+1+i+r}\frac{\mathrm{d}^i}{\mathrm{d}t^i}e^{t}\Big|_{t=x} \\
&= \sum_{r=0}^{n}\binom{n}{r}(-x\,y)^{n-r}e^{y}\sum_{i=0}^{r}A_r^i\,x^{\nu+1+i+r}e^{x}, \qquad (4.12)
\end{aligned}$$

which upon further simplification leads to:

$$\mathcal{D}_n(x,y,\nu) = (-x\,y)^n\,x^{\nu+1}\,e^{x+y}\sum_{r=0}^{n}\binom{n}{r}(-y)^{-r}\sum_{i=0}^{r}A_r^i\,x^i. \quad (4.13)$$

In a similar manner, we develop $\tilde{\mathcal{N}}_n(x,y,\nu)$ by using the Leibniz product rule and the SSF I with $(\mu,\nu,m,n) = (-2,\nu-1,0,0)$:

$$\tilde{\mathcal{N}}_n(x,y,\nu) = \frac{e^{-x-y}}{x^{\nu}\,y}\sum_{r=1}^{n}\binom{n}{r}\mathcal{D}_{n-r}(x,y,\nu)\,(x\,y)^r\sum_{s=0}^{r-1}\binom{r-1}{s}y^{-s}\sum_{i=0}^{s}A_s^i(-x)^i. \quad (4.14)$$

The coefficients A_r^i in (4.13) and A_s^i in (4.14) are given by equation (2.7).

Our approximations to $K_\nu(x,y)$ take the form:

$$\tilde{G}_n^{(1)}(x,y,\nu) = x^\nu \frac{\tilde{\mathcal{N}}_n(x,y,\nu)}{\mathcal{D}_n(x,y,\nu)}. \tag{4.15}$$

4.A.3 Numerical discussion

In [52], four numerical cases are presented and evaluated using a multiplicity of methods. With the approximations $\tilde{G}_n^{(1)}(x,y,\nu)$, we are capable of replicating these cases to the same pre-determined accuracy of $\pm 1 \times 10^{-10}$. We also show new results obtained with an accuracy of $\pm 1 \times 10^{-15}$ for which, in general, higher order transformations are required to achieve the higher pre-determined accuracy. For the region where $x \geq y$, we use the approximations $\tilde{G}_n^{(1)}(x,y,\nu)$ straightforwardly, and for the region where $x < y$, we use the inversion formula (4.4) and compute the approximations $\tilde{G}_n^{(1)}(y,x,-\nu)$ for the incomplete Bessel function $K_{-\nu}(y,x)$ and compute $K_\nu(2\,u)$ with the subroutine mikv.for from [40]. In Tables 4.1 and 4.2, we show the input variables x and y and parameter ν, the maximal order n of the transformation required, the corresponding approximation $\tilde{G}_n^{(1)}(x,y,\nu)$ of our FORTRAN 77 program, along with an approximation to the absolute error:

$$\text{Error} = \left| \tilde{G}_n^{(1)}(x,y,\nu) - \tilde{G}_{n-1}^{(1)}(x,y,\nu) \right|. \tag{4.16}$$

The four cases in [52] are:

Case 1. $x = 0.01$, $y = 4.00$, $\nu = 0(1)9$. We use (4.4) to invert x and y.

Case 2. $x = 4.95$, $y = 5.00$, $\nu = 2$. We again use (4.4) to invert x and y.

Case 3. $x = 10$, $y = 2$, $\nu = 6$. For this case, (4.4) is unnecessary, as $x > y$. We produce $K_6(10,2) = 0.00000\ 04150\ 04594\ 19162\ 55$, which is different from the “Accurate Value” $K_6(10, 2) = 0.00023\ 44186\ 32699$ given in [52] and the value obtained from the "Research of" [52] $K_6(10, 2) = 0.00023\ 44186\ 19816$. However, we suspect that there is a typographical error in [52] as numerical integration with Maple gives the: “Accurate Value” $K_6(10, 2) = 0.00000\ 04150\ 04594\ 23189\ 99$. Evidently, there is a disagreement between even the two accurate values, which leads us to suspect that the output in [52] does not correspond with $K_6(10, 2)$. Our approximation has an absolute error less than 10^{-10} with $n = 4$ and less than 10^{-15} with $n = 10$.

Case 4. $x = 3.1$, $y = 2.6$, $\nu = 5$.

Table 4.2 corresponds to a new table of values that we have compiled. This table shows the regions where the approximations $\tilde{G}_n^{(1)}(x, y, \nu)$ perform well, and also where a high order transformation is required to attain the desired pre-determined accuracy.

In Table 4.2, our approximations $\tilde{G}_n^{(1)}(x, y, \nu)$ are demonstrated on a wide range of x, y and ν. Simple values to approximate include rows 6, 7 and 8, where x and y are large. Challenging values to approximate include rows 1, 2, 12 and 13, where x and y are small. We note that in rows 9, 10 and 11, values of ν are real and non-integer. Equations (4.14) and (4.13) reveal that the computational complexity of the approximations $\tilde{G}_n^{(1)}(x, y, \nu)$ is independent of ν, which allows for an evaluation of $K_\nu(x, y)$ with real-, or even complex-, valued ν. In Table 4.2, we emphasize large values of ν. This is because the recurrence relation (4.2) is more stable in the downward direction for $x \geq y$. Therefore, since the values of ν vary from 0 to 16, the computation procedure would be more stable starting at the maximal ν and recurring downwards to maintain the pre-determined accuracy.

x	y	ν	n	$\tilde{G}_n^{(1)}(x,y,\nu)$	Error
0.01	4	0	10	0.2225310761289636(1)	0.57(-10)
0.01	4	1	7	0.2138941668493954(0)	0.96(-10)
0.01	4	2	5	0.5450346981126452(-1)	0.78(-10)
0.01	4	3	6	0.2325312150773913(-1)	0.21(-11)
0.01	4	4	7	0.1304275099607653(-1)	0.21(-11)
0.01	4	5	8	0.8567534990653542(-2)	0.31(-11)
0.01	4	6	9	0.6208676806589944(-2)	0.66(-11)
0.01	4	7	10	0.4801085238209789(-2)	0.19(-10)
0.01	4	8	11	0.3884072049500670(-2)	0.72(-10)
0.01	4	9	13	0.3246798003147811(-2)	0.62(-12)
4.95	5	2	16	0.1224999251036423(-4)	0.27(-10)
10.0	2	6	4	0.4150010642122851(-6)	0.29(-10)
3.1	2.6	5	12	0.5285042839881951(-3)	0.62(-10)

Table 4.1: Numerical Results for $\tilde{G}_n^{(1)}(x,y,\nu)$ for incomplete Bessel functions.

x	y	ν	n	$\tilde{G}_n^{(1)}(x,y,\nu)$	Error
1	1	8	48	0.1642584157597500(-1)	0.56(-15)
1	1	16	38	0.8393633437083270(-2)	0.68(-15)
5	5	4	18	0.8224363011631705(-5)	0.46(-15)
5	5	8	16	0.5034054653465547(-5)	0.60(-15)
5	5	16	13	0.2737360566898996(-5)	0.71(-15)
10	1	16	9	0.6565409733529793(-6)	0.69(-15)
10	5	16	8	0.1410826247065302(-7)	0.22(-15)
10	10	16	6	0.1204845014455500(-9)	0.20(-16)
1	5	1.6	18	0.4064821958669517(-2)	0.40(-15)
1	10	2.1	9	0.2137545215106365(-3)	0.56(-15)
5	10	3.5	16	0.1419478426782529(-6)	0.17(-15)
0.1	0.1	16	37	0.5113063337908691(-1)	0.93(-15)
0.5	0.5	12	46	0.3044667055799152(-1)	0.32(-15)

Table 4.2: Numerical Results for $\tilde{G}_n^{(1)}(x,y,\nu)$ for incomplete Bessel functions.

4.B Tail integrals of probability distributions

4.B.1 Definitions and basic properties

In this section, we define the normal distribution, the gamma distribution, the student's t-distribution, the inverse Gaussian distribution and Fisher's F distribution. For more details on these distributions and their properties, we refer the interested readers to [64, 65].

The normal distribution (Gaussian distribution) has the probability density function (PDF) given by:

$$f_N(x) = \frac{1}{\sqrt{2\,\pi\,\sigma^2}} \exp\left(-\frac{(x-\mu)^2}{2\,\sigma^2}\right) \qquad \text{for} \qquad -\infty < x < +\infty, \tag{4.17}$$

where μ denotes the mean of the distribution and σ^2 represents the variance.

By making the change of variable $z = \frac{x-\mu}{\sigma}$ the normal distribution reduces to the standard normal distribution where $\mu = 0$ and $\sigma^2 = 1$. In this case, the PDF is given by:

$$g_N(z) = \frac{1}{\sqrt{2\,\pi}} \exp\left(-\frac{z^2}{2}\right) \qquad \text{for} \qquad -\infty < z < +\infty. \tag{4.18}$$

The gamma distribution has the PDF:

$$f_g(x) = \frac{x^{a-1}\,e^{-\frac{x}{b}}}{\Gamma(a)\,b^a} \qquad \text{for} \qquad 0 < x < +\infty, \tag{4.19}$$

for which $a > 0$ and $b > 0$ are two parameters and Γ refers to the gamma function. The parameter a is responsible for the shape of the distribution whereas the parameter b affects the scale. The mean of the gamma distribution is $\mu = a\,b$ and the variance is $\sigma^2 = a\,b^2$. The gamma distribution is transformed to the exponential distribution by setting $a = 1$. It is also related to the chi-squared χ^2 distribution by setting $a = v/2$ and $b = 2$, where v is the number of degrees of freedom. Indeed, the gamma distribution also forms the heart of the noncentral gamma distribution studied in [66].

The student's t-distribution has the PDF:

$$f_t(x) = \frac{\Gamma(\frac{v+1}{2})}{\sqrt{v\,\pi}\,\Gamma\left(\frac{v}{2}\right)} \left(1 + \frac{x^2}{v}\right)^{-(\frac{v+1}{2})} \qquad \text{for} \qquad -\infty \,<\, x \,<\, +\infty, \quad (4.20)$$

where the parameter $v > 0$ stands for the number of degrees of freedom. For a sample size of n independent variables, the number of degrees of freedom is defined to be $v = n - 1$. The mean of the student's t-distribution is 0 and the variance is $\sigma^2 = \frac{v}{v-2}$ when $v > 2$, $\sigma^2 = \infty$ when $1 \,<\, v \,\leq\, 2$ and undefined otherwise. As v tends to infinity, the student's t-distribution converges toward the standard normal distribution.

The inverse Gaussian distribution has the PDF:

$$f_i(x) = \left(\frac{\lambda}{2\,\pi\,x^3}\right)^{\frac{1}{2}} \exp\left(-\frac{\lambda\,(x-\mu)^2}{2\,\mu^2\,x}\right) \qquad \text{for} \qquad 0 \,<\, x \,<\, +\infty, \quad (4.21)$$

where μ and λ are two parameters. The mean of the inverse Gaussian distribution is μ and the variance is $\sigma^2 = \frac{\mu^3}{\lambda}$.

Fisher's F distribution has the PDF:

$$f_F(x) = \frac{\Gamma\left(\frac{a+b}{2}\right)}{\Gamma\left(\frac{a}{2}\right)\,\Gamma\left(\frac{b}{2}\right)} \left(\frac{a}{b}\right)^{a/2} \frac{x^{\frac{a-2}{2}}}{\left(1 + \left(\frac{a}{b}\right)x\right)^{\frac{a+b}{2}}} \qquad \text{for} \qquad 0 \,<\, x \,<\, +\infty, \quad (4.22)$$

for which the integers a and b are two parameters. The mean of Fisher's F distribution is $\mu = \frac{b}{b-2}$ for $b > 2$ and the variance is $\sigma^2 = \frac{2\,b^2\,(a+b-2)}{a\,(b-2)^2\,(b-4)}$ for $b > 4$.

4.B.2 Computing the probability distributions

The objective of this section is to compute integral tails $\int_x^\infty f(t)\,\mathrm{d}t$ where $f(t)$ is a probability density function, using the algorithm for the $\tilde{G}_n^{(1)}$ transformation presented above.

The normal distribution

For simplicity, we first apply $G_n^{(1)}$ to the standard distribution. We derive the analytic expression of $\tilde{G}_n^{(1)}$ for the integral tail of the standard distribution, and then we make the change of variable $z = \frac{x-\mu}{\sigma}$ to obtain the analytic expression of $\tilde{G}_n^{(1)}$ for the integral tail of the normal distribution.

It is easy to show that the standard normal distribution PDF given by (4.18), satisfies a first order differential equation given by:

$$g_N(z) = p_1(z)\, g_N'(z), \tag{4.23}$$

where the coefficient $p_1(z)$ is given by:

$$p_1(z) \;=\; -\frac{1}{z} \;=\; -z^{-1} \quad \Rightarrow \quad \sigma_0 = -1 \quad (\text{see (3.9) for the definition of } \;\sigma_0)\,. \tag{4.24}$$

All the conditions required to apply the $G_n^{(1)}$ transformation to the standard distribution are satisfied. By Using SSF 1 with $(\mu,\nu,m,n) = (-2,-1,1,0)$ we obtain:

$$\begin{aligned}\mathcal{D}_n(z) &= \left(z^2\frac{\mathrm{d}}{\mathrm{d}z}\right)^n z\sqrt{2\pi}e^{z^2/2} \\ &= \frac{z^{1+n}}{g_N(z)}\sum_{i=0}^{n} A_n^i\, z^{2i},\end{aligned} \tag{4.25}$$

where the coefficients A_k^i are calculated using the recurrence relations in (2.7) with $(\mu, \nu, m, n) = (-2, -1, 1, 0)$.

Since the elements $\mathcal{D}_n(z)$ are now available, to evaluate the numerator $\tilde{\mathcal{N}}_n(z)$, we only need to evaluate the following:

$$\left(z^2 \frac{\mathrm{d}}{\mathrm{d}z}\right)^{r-1} \left(z^2 \frac{1}{\sqrt{2\,\pi}}\, e^{-\frac{z^2}{2}}\right). \tag{4.26}$$

We use the SSF 1 with $(\mu, \nu, m, n) = (-2, -2, 1, 0)$ to obtain:

$$\left(z^2 \frac{\mathrm{d}}{\mathrm{d}z}\right)^{r-1} \left(z^2 \frac{1}{\sqrt{2\,\pi}}\, e^{-\frac{z^2}{2}}\right) \;=\; z^{1+r}\, g_N(z) \sum_{i=0}^{r-1} B_{r-1}^i\, (-1)^i\, z^{2i}, \tag{4.27}$$

where the coefficients B_k^i are calculated using the recurrence relations in (2.7) with $(\mu, \nu, m, n) = (-2, -2, 1, 0)$.

Inserting these results into equation (3.17), we obtain:

$$\tilde{G}_n^{(1)}(z) \;=\; z\, g_N(z) \left[\frac{\displaystyle\sum_{r=1}^{n} \binom{n}{r} \sum_{i=0}^{n-r} A_{n-r}^i\, z^{2i} \sum_{j=0}^{r-1} B_{r-1}^j\, (-1)^j\, z^{2j}}{\displaystyle\sum_{k=0}^{n} A_n^k\, z^{2k}} \right]. \tag{4.28}$$

Upon the change of variables $z = \frac{x-\mu}{\sigma}$ to return to the general normal distribution, we obtain:

$$\tilde{G}_n^{(1)}(x) \;=\; (x-\mu)\, f_N(x) \left[\frac{\displaystyle\sum_{r=1}^{n} \binom{n}{r} \sum_{i=0}^{n-r} A_{n-r}^i\, \omega^i \sum_{j=0}^{r-1} B_{r-1}^j\, (-\omega)^j}{\displaystyle\sum_{k=0}^{n} A_n^k\, \omega^k} \right], \tag{4.29}$$

where $\omega = \left(\frac{x-\mu}{\sigma}\right)^2$.

In Table 4.3, we list values of the normal distribution. This table reproduces the numerical results presented in [26] for the normal distribution.

x	μ	σ	n	$\tilde{G}_n^{(1)}(x)$	ϵ_n	Maple values
1.2	0	1	48	.115069670221707(0)	.22(-15)	.115069670221708(0)
1.6	0	1	34	.547992916995587(-1)	.36(-15)	.547992916995579(-1)
2.0	0	1	28	.227501319481791(-1)	.79(-15)	.2275013194817920(-1)
3.0	0	1	19	.134989803163009(-2)	.41(-15)	.134989803163009(-2)
6.0	0	1	11	.986587645037697(-9)	.00(00)	.986587645037698(-9)
10.0	0	1	7	.761985302416049(-23)	.70(-15)	.7619853024160526(-23)
12.0	0	1	7	.177648211207767(-32)	.13(-15)	.1776482112077678(-32)
45.0	18	6	12	.339767312473006(-5)	.88(-15)	.339767312473006(-5)
54.2	2	25	28	.183989173418575(-1)	.28(-15)	.183989173418576(-1)
0.3	0	1	162	.382088577811118(0)	.30(-13)	.382088577811047(0)

Table 4.3: Numerical evaluation of the tail integral of the normal distribution by (4.29).

The gamma distribution

The probability density function $f_g(x)$ given by (4.19) satisfies the first order differential equation given by:

$$f_g(x) = p_1(x) f_g'(x), \tag{4.30}$$

where the coefficient $p_1(x)$ is given by:

$$p_1(x) = \frac{bx}{ab-b-x} = \sum_{n=0}^{\infty} \frac{-b^{n+1}(a-1)^n}{x^n} \quad \Rightarrow \quad \sigma_0 = 0. \tag{4.31}$$

Using SSF 1 with $(\mu, \nu, m, n) = (-2, a-1, 0, 0)$, we obtain:

$$\begin{aligned}\mathcal{D}_n(x) &= \left(x^2 \frac{\mathrm{d}}{\mathrm{d}x}\right)^n \Gamma(a)\, b^a\, x^{1-a} \exp\left(\frac{x}{b}\right) \\ &= \frac{x^n}{f_g(x)} \sum_{i=0}^{n} A_n^i \left(\frac{x}{b}\right)^i . \end{aligned} \tag{4.32}$$

For the numerator, we use $(\mu, \nu, m, n) = (-2, -a-1, 0, 0)$ to develop:

$$\left(x^2 \frac{\mathrm{d}}{\mathrm{d}x}\right)^{r-1} (x^2 f_g(x)) \;=\; x^{r+1} f_g(x) \sum_{i=0}^{r-1} B_{r-1}^i \left(-\frac{x}{b}\right)^i . \tag{4.33}$$

Inserting these results into equation (3.17), we obtain:

$$\tilde{G}_n^{(1)}(x) \;=\; x\, f_g(x) \left[\frac{\displaystyle\sum_{r=1}^{n} \binom{n}{r} \sum_{i=0}^{n-r} A_{n-r}^i \left(\frac{x}{b}\right)^i \sum_{j=0}^{r-1} B_{r-1}^j \left(-\frac{x}{b}\right)^j}{\displaystyle\sum_{k=0}^{n} A_n^k \left(\frac{x}{b}\right)^k} \right] . \tag{4.34}$$

In Table 4.4, we list values of the gamma distribution. This table reproduces the numerical results presented in [26] for the gamma distribution.

The student's t-distribution

The probability density function $f_t(x)$ given by (4.20) satisfies the first order differential equation given by:

$$f_t(x) = p_1(x) f_t'(x), \tag{4.35}$$

x	a	b	n	$\tilde{G}_n^{(1)}(x)$	ϵ_n	Maple values
13.0	7.000	2.0000	8	.526523622518000(0)	.00(00)	.526523622517999(0)
15.0	7.000	2.0000	8	.378154694323469(0)	.00(00)	.378154694323469(0)
20.0	7.000	2.0000	8	.130141420882482(0)	.00(00)	.130141420882482(0)
35.0	7.000	2.0000	8	.147001977487619(-2)	.00(00)	.147001977487619(-2)
40.0	7.000	2.0000	8	.255122495856300(-3)	.00(00)	.255122495856300(-3)
45.0	7.000	2.0000	8	.407935571774570(-4)	.00(00)	.407935571774571(-4)
50.0	7.000	2.0000	8	.610629446192788(-5)	.00(00)	.610629446192790(-5)
60.0	7.000	2.0000	8	.117319420023469(-6)	.00(00)	.117319420023469(-6)
120.0	7.000	2.0000	7	.629224133230851(-18)	.38(-15)	.629224133230850(-18)
12.0	2.000	3.0000	3	.915781944436709(-1)	.00(00)	.915781944436709(-1)
25.5	4.430	2.0230	11	.251747197371780(-2)	.15(-13)	.251747197371771(-2)
45.0	5.432	4.5432	13	.453930946920760(-1)	.24(-13)	.453930946920784(-1)
14.0	1.111	9.0000	45	.245873088348530(0)	.33(-15)	.245873088348520(0)

Table 4.4: Numerical evaluation of the tail integral of the gamma distribution by (4.34).

where the coefficient $p_1(x)$ is given by:

$$p_1(x) \;=\; -\frac{x^2+v}{x(v+1)} \;=\; x\left(-\frac{1}{v+1} - \frac{v}{(v+1)x^2}\right) \quad \Rightarrow \quad \sigma_0 = 1. \tag{4.36}$$

The $G_n^{(1)}$ transformation then gives:

$$\tilde{G}_n^{(1)}(x) \;=\; x f_t(x) \left[\frac{\displaystyle\sum_{r=1}^{n} \binom{n}{r} \sum_{i=0}^{n-r} A_{n-r}^{i}\,(\omega)_i\, z^i \sum_{j=0}^{r-1} B_{r-1}^{j}\,(-\omega)_j\, z^j}{\displaystyle\sum_{k=0}^{n} A_n^k\,(\omega)_k\, z^k} \right], \tag{4.37}$$

where $\omega = -\frac{v+1}{2}$, $z = -\frac{2\,x^2}{v+x^2}$ and $(x)_n = x(x+1)\cdots(x+n-1)$ is a Pochhammer symbol, and where A_k^i are the coefficients of the SSF 1 with $(\mu,\nu,m,n) = (-2,1,1,0)$ and the B_k^i are the coefficients of the SSF 1 with $(\mu,\nu,m,n) = (-2,-2,1,0)$.

In Table 4.5, we list values of the student's t-distribution. This table reproduces the numerical results presented in [26] for the student's t-distribution.

x	v	n	$\tilde{G}_n^{(1)}(x)$	ϵ_n	Maple values
1.812	10	28	.500376310329719(-1)	.17(-11)	.500376310329236(-1)
2.228	10	26	.250058859084132(-1)	.16(-11)	.250058859085556(-1)
3.169	10	19	.500231668217826(-2)	.57(-12)	.500231668219242(-2)
4.587	10	21	.499918645935931(-3)	.62(-13)	.499918645938171(-3)
6.927	20	12	.500032563506471(-6)	.46(-13)	.500032563506499(-6)
5.449	60	11	.499901999489751(-6)	.85(-14)	.499901999489723(-6)
3.373	120	21	.500752580750085(-3)	.45(-13)	.500752580749990(-3)
20.0	120	11	.255269495907817(-39)	.16(-15)	.255269495907814(-39)
12.49	45	9	.158367022750732(-15)	.37(-14)	.158813184049678(-15)
5.402	5	15	.146875507310926(-2)	.40(-11)	.146875507309968(-2)

Table 4.5: Numerical evaluation of the tail integral of the student's t-distribution by (4.37).

The inverse Gaussian distribution

The probability density function $f_i(x)$ given by (4.21) satisfies the first order differential equation given by:

$$f_i(x) \;=\; p_1(x) f_i'(x), \tag{4.38}$$

where the coefficient $p_1(x)$ is given by:

$$p_1(x) \;=\; \frac{-2\mu^2 x^2}{\lambda x^2 + 3\mu^2 x - \lambda\mu^2} = \left(-\frac{2\mu^2}{\lambda} + \frac{6\mu^2}{\lambda^2 x} - \ldots\right) \quad \Rightarrow \quad \sigma_0 = 0. \tag{4.39}$$

The $G_n^{(1)}$ transformation then gives:

$$\tilde{G}_n^{(1)}(x) = \frac{2\,x^2\,f_i(x)}{\lambda} \times \left[\frac{\displaystyle\sum_{r=1}^{n} \binom{n}{r} (-1)^r \sum_{k=0}^{n-r} \binom{n-r}{k} (-\omega)^k \sum_{i=0}^{k} A_k^i\, z^i \sum_{q=0}^{r-1} \binom{r-1}{q} \omega^q \sum_{l=0}^{q} B_q^l\,(-z)^l}{\displaystyle\sum_{m=0}^{n} \binom{n}{m} (-\omega)^m \sum_{p=0}^{m} A_m^p\, z^p} \right], \tag{4.40}$$

where $\omega = \frac{2\,x}{\lambda}$ and $z = \frac{\lambda\,x}{2\,\mu^2}$, and where A_k^i are the coefficients of the SSF 1 with $(\mu, \nu, m, n) = (-2, -\frac{3}{2}, 0, 0)$ and the B_k^i are the coefficients of the SSF 1 with $(-2, -\frac{1}{2}, 1, 0)$.

In Table 4.6, we list values of the inverse Gaussian distribution. This table reproduces the numerical results presented in [26] for the inverse Gaussian distribution.

x	μ	λ	n	$\tilde{G}_n^{(1)}(x)$	ϵ_n	Maple values
1.50	1.00	1.00	107	.189232007000019(0)	.92(-15)	.189232007000020(0)
2.00	1.00	1.00	82	.114524574013992(0)	.43(-15)	.114524574013993(0)
3.00	1.00	1.00	61	.468120792572114(-1)	.63(-15)	.468120792572116(-1)
4.50	1.00	1.00	42	.143011829460930(-1)	.00(00)	.143011829460931(-1)
6.00	1.00	1.00	35	.484988213370218(-2)	.00(00)	.484988213370217(-2)
10.00	1.00	1.00	36	.350414537208826(-3)	.65(-15)	.350414537208819(-3)
16.00	1.00	1.00	24	.943916863494728(-5)	.39(-15)	.943916863494723(-5)
32.00	1.00	1.00	16	.122006566375975(-8)	.72(-15)	.122006566375975(-8)
24.00	2.00	4.00	27	.510429100438049(-6)	.14(-15)	.510429100438016(-6)
33.46	4.54	2.78	40	.621975008388134(-2)	.72(-15)	.621975008388144(-2)
23.00	6.54	6.00	55	.333636164607366(-1)	.71(-15)	.333636164607370(-1)
0.50	1.00	1.00	165	.635024451788276(0)	.49(-11)	.635024451827040(0)

Table 4.6: Numerical evaluation of the tail integral of the inverse Gaussian distribution by (4.40).

Fisher's F distribution

The probability density function $f_F(x)$ given by (4.22) satisfies the first order differential equation given by:

$$f_F(x) \;=\; p_1(x) f_F'(x), \tag{4.41}$$

where the coefficient $p_1(x)$ is given by:

$$p_1(x) \;=\; -\frac{2ax^2+2bx}{(2a+ab)x+2b-ab} = x\left(-\frac{2}{2+b} - \frac{2b(b+a)}{(2+b)^2 ax} - \dots\right) \quad \Rightarrow \quad \sigma_0 = 1. \tag{4.42}$$

The $G_n^{(1)}$ transformation then gives:

$$\tilde{G}_n^{(1)}(x) \;=\; x f_F(x) \left[\frac{\displaystyle\sum_{r=1}^{n} \binom{n}{r} \sum_{i=0}^{n-r} A_{n-r}^{i}\,(\omega)_i\, z^i \sum_{j=0}^{r-1} B_{r-1}^{j}\,(-\omega)_j\, z^j}{\displaystyle\sum_{k=0}^{n} A_n^k\,(\omega)_k\, z^k}\right], \tag{4.43}$$

where $\omega = -\frac{a+b}{2}$ and $z = -\frac{a\,x}{a\,x+b}$, and where A_k^i are the coefficients of the SSF 1 with $(\mu,\nu,m,n) = (-2, \frac{a}{2}, 0, 0)$ and the B_k^i are the coefficients of the SSF 1 with $(-2, -\frac{a+2}{2}, 0, 0)$.

In Table 4.7, we list values of Fisher's F distribution. This table reproduces the numerical results presented in [26] for Fisher's F distribution.

4.B.3 Numerical discussion

The SSF 1 greatly simplifies the computation of the algorithm when using a FORTRAN compiler due to the recurrence relations (2.7) satisfied by the coefficients A_k^i. This internal recursion leads to a considerable gain in the cal-

x	a	b	n	$\tilde{G}_n^{(1)}(x)$	ϵ_n	Maple values
4.190	3	4	14	.100029643896889(0)	.68(-13)	.100029643896895(0)
6.590	3	4	12	.500168891790474(-1)	.11(-12)	.500168891790405(-1)
9.980	3	4	11	.249965339234578(-1)	.31(-13)	.249965339234568(-1)
16.70	3	4	9	.999383733001448(-2)	.17(-13)	.999383733001462(-2)
5.750	5	1	10	.306042577763992(0)	.15(-12)	.306042577763857(0)
3.340	1	1	18	.318737836141563(0)	.43(-12)	.318737836141636(0)
23.23	10	5	7	.142310351602081(-2)	.17(-13)	.142310351602084(-2)
12.05	8	3	6	.325796489130341(-1)	.53(-14)	.325796489130337(-1)

Table 4.7: Numerical evaluation of the tail integral of Fisher's F distribution by (4.43).

culation times compared to the use of a method to solve the linear system (3.9). In addition, the recurrence relations (2.7) allow us to stop the calculation as soon as the desired precision is attained. That is, we calculate the approximation $\tilde{G}_{n+1}^{(1)}$ only if the precision attained by $\tilde{G}_n^{(1)}$ is insufficient. We use the following test based on an approximation to the relative error as a stopping criterion in the calculations:

$$\epsilon_n = \left| \frac{\tilde{G}_n^{(1)}(x) - \tilde{G}_{n-1}^{(1)}(x)}{\tilde{G}_n^{(1)}(x)} \right| \leq \epsilon, \tag{4.44}$$

where ϵ is defined according to the desired degree of precision. In all our calculations, ϵ is set at 10^{-15}.

In general, the test of accuracy (4.44) works well. However, in certain instances, when the behavior of the sequence of approximations $\{\tilde{G}_n^{(1)}(x)\}$ is unstable and after an optimal order of approximation, the error will only grow larger (see Figures 4.1(a) and 4.1(b) and their corresponding Tables 4.8 and 4.9). In such a situation, we must therefore stop the calculation, knowing that the error will only grow larger. The stopping criterion in such an instance is determined by the following test:

$$\varrho_i = \left| \frac{\tilde{G}^{(1)}_{n-i}(x) - \tilde{G}^{(1)}_{n-1-i}(x)}{\tilde{G}^{(1)}_{n-1-i}(x) - \tilde{G}^{(1)}_{n-2-i}(x)} \right| > 1 \qquad \text{for} \qquad i = 0, 1, 2, \ldots. \tag{4.45}$$

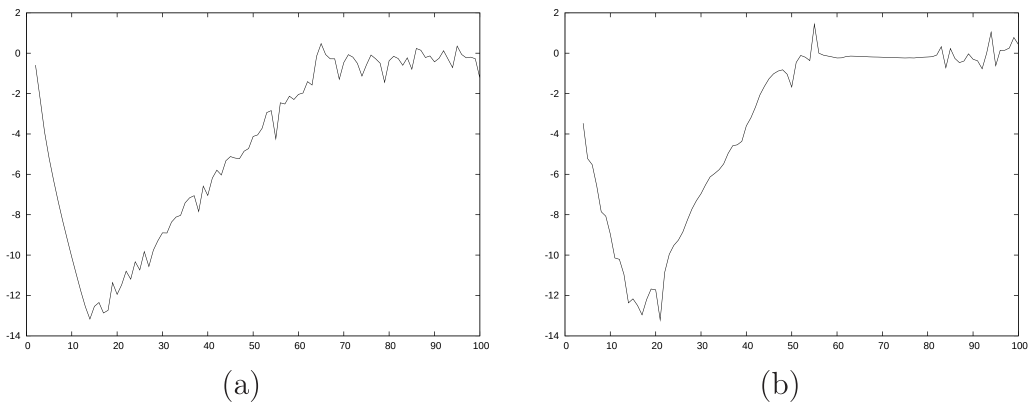

Figure 4.1: Plot of $\log_{10}(\epsilon_n)$ given by (4.44) as a function of the order n of the approximations $\tilde{G}^{(1)}_n(x)$ for (a) Fisher's F distribution with $x = 4.19$, $a = 3$, and $b = 4$ (corresponds to Table 4.8) and for (b) the student's t-distribution with $x = 4.587$ and $v = 10$ (corresponds to Table 4.9).

We found that $\varrho_0 > 1$ was a sufficient stopping criterion for Fisher's F and the gamma distributions. For the student's t-distribution, $\varrho_i > 1$ for $i = 0, 1, 2$ are required in order to achieve the best numerical result. For Fisher's F distribution, when $\varrho_0 > 1$ is used, we found that the $\tilde{G}^{(1)}_{n-1}(x)$ term gives the best result. In Table 4.8, we have $\varrho_0 > 1$ at $n = 15$ and the best approximation is given by $\tilde{G}^{(1)}_{14}(x)$.

For the gamma distribution, we found that the $\tilde{G}^{(1)}_n(x)$ term gives the best result. Using $\varrho_i > 1$ for $i = 0, 1, 2$ for the student's t-distribution, we found that the $\tilde{G}^{(1)}_{n-3}(x)$ term gives the best result. In Table 4.9, we have $\varrho_i > 1$ for $i = 0, 1, 2$ at $n = 24$ and the best approximation is given by $\tilde{G}^{(1)}_{21}(x)$.

Figure 4.1 shows representative plots of $\log_{10}(\epsilon_n)$ for (a) Fisher's F distribution and for (b) the student's t-distribution. Figure 4.1 (a) shows a typical error curve which allows the test for $\varrho_0 > 1$ to achieve the optimal approximation. In contrast, Figure 4.1 (b) shows a typical error curve which prevents the test for $\varrho_0 > 1$ from achieving the optimal approximation. Heuristically speaking, the irregularities in the sequence of relative errors present in Figure 4.1 (b) but absent in Figure 4.1 (a) cause the test for $\varrho_0 > 1$ to stop the algorithm premature of the optimal approximation. After analysis of numerous similar plots, we find that only the student's t-distribution requires additional test.

n	$\tilde{G}_n^{(1)}$	ϵ_n	ϱ_0
⋮	⋮	⋮	⋮
7	.100 029 643 323 462(0)	.46(-07)	.09(0)
8	.100 029 643 826 732(0)	.50(-08)	.10(0)
9	.100 029 643 887 614(0)	.60(-09)	.12(0)
10	.100 029 643 895 591(0)	.79(-10)	.13(0)
11	.100 029 643 896 704(0)	.11(-10)	.13(0)
12	.100 029 643 896 869(0)	.16(-11)	.14(0)
13	.100 029 643 896 896(0)	.27(-12)	.16(0)
14	.100 029 643 896 889(0)	.68(-13)	.24(0)
15	.100 029 643 896 918(0)	.28(-12)	.42(1)
16	.100 029 643 896 873(0)	.44(-12)	.15(1)
17	.100 029 643 896 887(0)	.13(-12)	.30(0)
⋮	⋮	⋮	⋮
59	.978 730 933 819 339(-1)	.50(-02)	.68(0)
60	.987 747 825 057 981(-1)	.91(-02)	.18(1)
61	.977 349 542 823 236(-1)	.10(-01)	.11(1)
62	.940 746 788 876 968(-1)	.38(-01)	.35(1)
⋮	⋮	⋮	⋮

Table 4.8: Error table for Fisher's F distribution for $x = 4.19$ and $a = 3$ and $b = 4$ by (4.43). $\tilde{G}_{14}^{(1)}$ is the approximation obtained from our algorithm.

Generally speaking, the accuracy improves as the order n in the $\tilde{G}_n^{(1)}$ trans-

n	$\tilde{G}_n^{(1)}$	ϵ_n	ϱ_0	ϱ_1	ϱ_2
$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$
16	.499 918 645 938 139(-3)	.32(-12)	.48(0)	.16(1)	.03(0)
17	.499 918 645 938 192(-3)	.11(-12)	.33(0)	.48(0)	.16(1)
18	.499 918 645 937 877(-3)	.63(-12)	.59(1)	.33(0)	.48(0)
19	.499 918 645 936 838(-3)	.21(-11)	.33(1)	.59(1)	.33(0)
20	.499 918 645 935 900(-3)	.19(-11)	.90(0)	.33(1)	.59(1)
21	.499 918 645 935 931(-3)	.62(-13)	.03(0)	.90(0)	.33(1)
22	.499 918 645 928 744(-3)	.14(-10)	.23(3)	.03(0)	.90(0)
23	.499 918 645 876 004(-3)	.11(-09)	.73(1)	.23(3)	.03(0)
24	.499 918 645 725 138(-3)	.30(-09)	.29(1)	.73(1)	.23(3)
25	.499 918 645 449 595(-3)	.55(-09)	.18(1)	.29(1)	.73(1)
26	.499 918 644 750 484(-3)	.14(-08)	.25(1)	.18(1)	.29(1)
$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$
49	.906 689 643 668 337(-3)	.91(-01)	.65(0)	.14(1)	.16(1)
50	.925 745 751 045 273(-3)	.21(-01)	.23(0)	.65(0)	.14(1)
51	.143 490 605 510 311(-2)	.35(00)	.27(2)	.23(0)	.65(0)
$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$

Table 4.9: Error table for the student's t-distribution for $x = 4.587$ and $v = 10$ by (4.37). $\tilde{G}_{21}^{(1)}$ is the approximation obtained from our algorithm.

formation increases. However, after a certain value of iteration depending on the arguments provided, overflow occurs. The program returns the message NaN (Not a Number) due to the divergent nature of the coefficients in the SSF 1. In such a situation, we used the following stopping criteria in our algorithm:

$$\tilde{\mathcal{N}}_n(x) > \text{Huge} \qquad \text{or} \qquad \mathcal{D}_n(x) > \text{Huge}. \tag{4.46}$$

The value of Huge is chosen close, but not equal to the largest real number that can be stored by the machine. We chose the value 10^{300} in our program. In this case, we pick the value $\tilde{G}_{n-1}^{(1)}(x)$ as the best result.

Tables 4.8 and 4.9 show sequences of values obtained at each iteration of the

$\tilde{G}_n^{(1)}$ transformation for the F distribution and the t distribution respectively. From these tables, we can clearly see how the use of the $\varrho_i > 1$ test helped us reach the most accurate numerical results.

Tables 4.3 to 4.7 reproduce all of the numerical results presented in [26].

In the calculation presented in Table 4.4, it is important to note that for integer values of a, the integrand has a closed-form anti-derivative, thus $\tilde{G}_a^{(1)}(x)$ is equal to the true value. For the numerical calculation of the gamma function we use the subroutine Mgamma.for [40]. In this table, we also add additional values with non-integer parameters to show how our method performs when no closed-form anti-derivatives are known.

When we compare our numerical results with those obtained in [26], all values agree except for the seventh entry in Table 1 in [26]. For this entry, we find .1776482112077677(−32) which is in agreement with the value that we obtained using the symbolic programming language Maple .177648211207767(−32). The value given in [26] is 0.367097(−50) and we suspect this is a typographical error.

We also used Maple to compute the tail probabilities with an accuracy of 15 correct digits and the values obtained are listed in Tables 4.3-4.7 in the columns 'Maple values.' The evalf[15] command of Maple was used for a straightforward calculation of the integral tails, where the [15] denotes the number of digits Maple will return in the computed expression. A straightforward calculation in Maple consists of entering the infinite-range integrals symbolically and recuperating a numerical value, whether the integral has a closed-form antiderivative or not.

Chapter 5

Analysis of Convergence Properties

In this chapter, we study the convergence properties of the $G_n^{(1)}$ transformation. We begin by sharpening the asymptotics of the $G_n^{(1)}$ transformation, first proved in [13]. Then, with the explicit expression from the algorithmic form for the $G_n^{(1)}$ transformation and with a specific form for the integrand, we study the rational and Padé approximants [67] given by the $G_n^{(1)}$ transformation. With this connection established, we use the method of Viskovatov to transform the rational and Padé approximants with an accuracy-through-order condition into continued fractions. Upon extrapolation to the limit, through convergence theorems on continued fractions, we infer convergence of the $G_n^{(1)}$ transformation applied to the normal and gamma distributions.

5.A Connection with rational and Padé approximants

As can be seen from equations (4.29), (4.34), (4.37), (4.40) and (4.43), the approximations $\tilde{G}_n^{(1)}(x)$ to the tail probabilities all have similar forms. To study the forms more closely, including their connection with other approximation methods, we require the following Lemma.

Lemma 5.1: *Let $f(x)$ have the form:*

$$f(x) = A\,x^{\mu} e^{r(x)}, \tag{5.1}$$

where $A \in \mathbb{R}/0$, $\mu \in \mathbb{R}$ and $r(x) \in \mathbb{R}[x]$ with $\deg(r(x)) = r_0 \geq 0$. Then, for $i = 0, 1, \ldots,$ and for $\alpha \in \mathbb{R}$ and $\beta \in \mathbb{R}$, it follows that:

$$\left(x^{\alpha+1}\frac{\mathrm{d}}{\mathrm{d}x}\right)^i (x^{\beta} f(x)) = x^{\alpha\, i+\beta} f(x) s_i(x), \tag{5.2a}$$

$$\left(x^{\alpha+1}\frac{\mathrm{d}}{\mathrm{d}x}\right)^i \left(\frac{x^{\beta}}{f(x)}\right) = \frac{x^{\alpha\, i+\beta}}{f(x)} t_i(x), \tag{5.2b}$$

where $s_i(x) \in \mathbb{R}[x]$ with $\deg(s_i(x)) = i\,r_0$ and $t_i(x) \in \mathbb{R}[x]$ with $\deg(t_i(x)) = i\,r_0$.

Proof. The demonstration of either (5.2a) or (5.2b) is sufficient, as $\frac{1}{f(x)} = A^{-1}x^{-\mu}e^{-r(x)}$ is still in the form of (5.1) if, for example, we take $B = A^{-1}$, $\nu = -\mu$ and $s(x) = -r(x)$.

To prove (5.2a), we begin with $i = 0$. In this case $s_0(x) = 1$. For $i = 1$:

$$
\begin{aligned}
x^{\alpha+1}\frac{\mathrm{d}}{\mathrm{d}x}(x^{\beta} f(x)) &= x^{\alpha+1}\left[A(\beta+\mu)x^{\beta+\mu-1} + A x^{\beta+\mu} r'(x)\right] e^{r(x)} \\
&= x^{\alpha+\beta} A\, x^{\mu} e^{r(x)} \left[(\beta+\mu) + x\, r'(x)\right] \\
&= x^{\alpha+\beta} f(x) s_1(x), \qquad (5.3)
\end{aligned}
$$

where $s_1(x) \in \mathbb{R}[x]$ with $\deg(s_1(x)) = r_0$. For $i > 1$, the proof follows by induction:

$$
\begin{aligned}
\left(x^{\alpha+1}\frac{\mathrm{d}}{\mathrm{d}x}\right)(x^{\beta+\alpha(i-1)} f(x) s_{i-1}(x)) &= x^{\alpha(i-1)} s_{i-1}(x) \left(x^{\alpha+1}\frac{\mathrm{d}}{\mathrm{d}x}\right)(x^{\beta} f(x)) \\
&\quad + x^{\beta} f(x) \left(x^{\alpha+1}\frac{\mathrm{d}}{\mathrm{d}x}\right)(x^{\alpha(i-1)} s_{i-1}(x)) \\
&= x^{\alpha(i-1)} s_{i-1}(x) x^{\alpha+\beta} f(x) s_1(x) \\
&\quad + x^{\beta} f(x)(\alpha(i-1)x^{\alpha\, i} s_{i-1}(x) + x^{\alpha\, i+1} s'_{i-1}(x)) \\
&= x^{\alpha\, i+\beta} f(x) s_{i-1}(x) s_1(x) \\
&\quad + x^{\alpha\, i+\beta} f(x)(\alpha(i-1) s_{i-1}(x) + x\, s'_{i-1}(x)) \\
&= x^{\alpha\, i+\beta} f(x) s_i(x), \qquad (5.4)
\end{aligned}
$$

where $s_i(x) \in \mathbb{R}[x]$ with $\deg(s_i(x)) = i\, r_0$. □

Lemma 5.2: *Let $\omega(x)$ be such that:*

$$
\omega(x) \sim A\, x^{\mu} e^{r(x)}, \quad \text{as} \quad x \to \infty, \qquad (5.5)
$$

where $A \in \mathbb{R}/0$, $\mu \in \mathbb{R}$ and $r(x) \in \mathbb{R}[x]$ with $\deg(r(x)) = r_0 \geq 0$. Then, for

$n = 0, 1, \ldots,$ and for $\alpha \in \mathbb{R}$, it follows that:

$$\frac{\left(x^{\alpha+1}\frac{\mathrm{d}}{\mathrm{d}x}\right)^{n-1}\left(\frac{1}{\omega(x)}\right)}{\left(x^{\alpha+1}\frac{\mathrm{d}}{\mathrm{d}x}\right)^{n}\left(\frac{1}{\omega(x)}\right)} \sim \frac{\omega_n}{x^{\alpha+r_0}}, \quad \text{as} \quad x \to \infty, \tag{5.6}$$

where $\omega_n \in \mathbb{R}$ is a constant.

Proof. By Lemma 5.1, since $\omega(x) \sim f(x)$, where $f(x)$ is given in (5.1), the left-hand side of (5.6) is then:

$$\begin{aligned}
\frac{\left(x^{\alpha+1}\frac{\mathrm{d}}{\mathrm{d}x}\right)^{n-1}\left(\frac{1}{\omega(x)}\right)}{\left(x^{\alpha+1}\frac{\mathrm{d}}{\mathrm{d}x}\right)^{n}\left(\frac{1}{\omega(x)}\right)} &\sim \frac{\left(x^{\alpha+1}\frac{\mathrm{d}}{\mathrm{d}x}\right)^{n-1}\left(\frac{1}{f(x)}\right)}{\left(x^{\alpha+1}\frac{\mathrm{d}}{\mathrm{d}x}\right)^{n}\left(\frac{1}{f(x)}\right)}, \quad \text{as} \quad x \to \infty, && (5.7)\\
&= \frac{\dfrac{x^{\alpha(n-1)}}{f(x)}t_{n-1}(x)}{\dfrac{x^{\alpha n}}{f(x)}t_n(x)}, && (5.8)\\
&= \frac{t_{n-1}(x)}{x^{\alpha}\, t_n(x)}, && (5.9)\\
&\sim \frac{\omega_n}{x^{\alpha+r_0}}, \quad \text{as} \quad x \to \infty, && (5.10)
\end{aligned}$$

where $\omega_n \in \mathbb{R}$ is a constant whose dependence on n is highlighted. □

We now have the tools to derive asymptotic error estimates for the $G_n^{(1)}$ transformation. However, we do this with a generalized notation. Let $F(x) = \int_0^x f(t)\,\mathrm{d}t$ and let $I[f] = \lim_{x\to\infty} F(x)$. Let also:

$$I[f] - F(x) \sim \omega(x) \sum_{i=0}^{\infty} \frac{\beta_i}{x^{\alpha i}} \qquad \text{as} \qquad x \to \infty, \tag{5.11}$$

where $\alpha \in \mathbb{R}^+$ and $\omega : \mathbb{R} \to \mathbb{R}$. Then, using the analogous annihilation operator to the one used in (3.17), we obtain the approximations:

$$G_n^{(1,\alpha)}(x) = \frac{\left(x^{\alpha+1}\dfrac{\mathrm{d}}{\mathrm{d}x}\right)^n \left(\dfrac{F(x)}{\omega(x)}\right)}{\left(x^{\alpha+1}\dfrac{\mathrm{d}}{\mathrm{d}x}\right)^n \left(\dfrac{1}{\omega(x)}\right)}. \tag{5.12}$$

It is self-evident that when $\omega(x) = x^{\sigma_0} f(x)$, then $G_n^{(1,1)}(x) = G_n^{(1)}(x)$. We now develop the asymptotic error estimate for this generalized $G_n^{(1,\alpha)}$ transformation.

Theorem 5.1: *Let* $\lim_{x\to\infty} F(x) = I[f]$. *Let* $I[f] - F(x)$ *have the asymptotic expansion given by* (5.11) *where* $\omega(x)$ *is such that* (5.5) *holds. Then the approximations* $G_n^{(1,\alpha)}(x)$ *given in* (5.12) *satisfy:*

$$\frac{I[f] - G_n^{(1,\alpha)}(x)}{I[f] - G_{n-1}^{(1,\alpha)}(x)} = \mathcal{O}\left(\frac{1}{x^{\alpha+r_0}}\right) \quad \text{as} \quad x \to \infty. \tag{5.13}$$

Proof. Using (5.12), the ratio (5.13) is given by:

$$\frac{I[f] - G_n^{(1,\alpha)}(x)}{I[f] - G_{n-1}^{(1,\alpha)}(x)} = \frac{\left(x^{\alpha+1}\dfrac{\mathrm{d}}{\mathrm{d}x}\right)^n \left(\dfrac{I[f] - F(x)}{\omega(x)}\right)}{\left(x^{\alpha+1}\dfrac{\mathrm{d}}{\mathrm{d}x}\right)^{n-1} \left(\dfrac{I[f] - F(x)}{\omega(x)}\right)} \tag{5.14}$$

$$\times \frac{\left(x^{\alpha+1}\dfrac{\mathrm{d}}{\mathrm{d}x}\right)^{n-1} \left(\dfrac{1}{\omega(x)}\right)}{\left(x^{\alpha+1}\dfrac{\mathrm{d}}{\mathrm{d}x}\right)^n \left(\dfrac{1}{\omega(x)}\right)}, \tag{5.15}$$

since $I[f]$ is a constant and since $\left(x^{\alpha+1}\dfrac{\mathrm{d}}{\mathrm{d}x}\right)$ is a linear operator. We investigate both ratios separately. Firstly, from the asymptotic condition (5.11), the first ratio is asymptotic to a constant:

$$\frac{\left(x^{\alpha+1}\frac{\mathrm{d}}{\mathrm{d}x}\right)^{n}\left(\frac{I[f]-F(x)}{\omega(x)}\right)}{\left(x^{\alpha+1}\frac{\mathrm{d}}{\mathrm{d}x}\right)^{n-1}\left(\frac{I[f]-F(x)}{\omega(x)}\right)} \sim \frac{\left(x^{\alpha+1}\frac{\mathrm{d}}{\mathrm{d}x}\right)^{n}\sum_{i=0}^{\infty}\frac{\beta_i}{x^{\alpha i}}}{\left(x^{\alpha+1}\frac{\mathrm{d}}{\mathrm{d}x}\right)^{n-1}\sum_{i=0}^{\infty}\frac{\beta_i}{x^{\alpha i}}} \quad \text{as} \quad x\to\infty, \tag{5.16}$$

$$= \frac{\displaystyle\sum_{i=n}^{\infty}\frac{(-\alpha)^n i!\beta_i}{(i-n)!x^{\alpha(i-n)}}}{\displaystyle\sum_{i=n-1}^{\infty}\frac{(-\alpha)^{n-1}i!\beta_i}{(i-n+1)!x^{\alpha(i-n+1)}}}, \tag{5.17}$$

$$\sim \frac{(-\alpha)^n n!\beta_n}{(-\alpha)^{n-1}(n-1)!\beta_{n-1}} \quad \text{as} \quad x\to\infty, \tag{5.18}$$

$$= -\frac{\alpha\, n\, \beta_n}{\beta_{n-1}}. \tag{5.19}$$

And from Lemma 5.2, the second ratio is asymptotic to:

$$\frac{\left(x^{\alpha+1}\frac{\mathrm{d}}{\mathrm{d}x}\right)^{n-1}\left(\frac{1}{\omega(x)}\right)}{\left(x^{\alpha+1}\frac{\mathrm{d}}{\mathrm{d}x}\right)^{n}\left(\frac{1}{\omega(x)}\right)} \sim \frac{\omega_n}{x^{\alpha+r_0}}, \quad \text{as} \quad x\to\infty. \tag{5.20}$$

Combining these ratios, it is trivial to obtain the asymptotic condition (5.13).

□

By induction on the order n of the transformation, it is equivalent to state:

$$\frac{I[f]}{\omega(x)} - \frac{G_n^{(1,\alpha)}(x)}{\omega(x)} = \mathcal{O}\left(\frac{1}{x^{(\alpha+r_0)n}}\right) \quad \text{as} \quad x\to\infty. \tag{5.21}$$

or for the $\tilde{G}_n^{(1,\alpha)}(x)$ transformation defined by $\tilde{G}_n^{(1,\alpha)}(x) = G_n^{(1,\alpha)}(x) - F(x)$:

$$\frac{\tilde{G}_n^{(1,\alpha)}(x)}{\omega(x)} - \frac{\int_x^\infty f(t)\,\mathrm{d}t}{\omega(x)} = \mathcal{O}\left(\frac{1}{x^{(\alpha+r_0)n}}\right) \quad \text{as} \quad x \to \infty. \tag{5.22}$$

With these tools, we are able to describe the general form of the approximations $\tilde{G}_n^{(1)}(x)$ to $\int_x^\infty f(t)\,\mathrm{d}t$ for integrals whose integrands are of the form (5.1).

Theorem 5.2: *Let $f(x)$ be integrable at infinity (i.e. $\left|\int_x^\infty f(t)\,\mathrm{d}t\right| < \infty$ for some $x \in \mathbb{R}$) and have the general form prescribed by* (5.1)*. The approximations $\tilde{G}_n^{(1,\alpha)}(x)$ to $\int_x^\infty f(t)\,\mathrm{d}t$ take the form:*

$$\tilde{G}_n^{(1,\alpha)}(x) = x\,f(x)\frac{a_n(x)}{b_n(x)}, \tag{5.23}$$

where $a_n(x) \in \mathbb{R}[x]$ with $\deg(a_n(x)) \leq (n-1)\,r_0$ and $b_n(x) \in \mathbb{R}[x]$ with $\deg(b_n(x)) = n\,r_0$.

Proof. The function (5.1) satisfies:

$$f(x) = p_1(x)f'(x), \tag{5.24}$$

where:

$$p_1(x) = \frac{x}{\mu + x\,r'(x)} \sim x^{1-r_0}\sum_{i=0}^{\infty}\frac{\alpha_i}{x^i} \qquad \text{as} \qquad x \to \infty. \tag{5.25}$$

Therefore, $f(x) \in \mathbf{B}^{(1)}$ and the approximations $\tilde{G}_n^{(1,\alpha)}(x)$ can be constructed as in section 3.B.

Applying Lemma 5.1 to (3.17) or its generalization (5.12), we obtain:

$$\begin{aligned}
\tilde{G}_n^{(1,\alpha)}(x) &= \frac{\sum_{r=1}^{n} \binom{n}{r} \mathcal{D}_{n-r}(x) \, \left(x^{\alpha+1} \frac{\mathrm{d}}{\mathrm{d}x}\right)^{r-1} (x^{\alpha+1} f(x))}{\mathcal{D}_n(x)} \\
&= \frac{\sum_{r=1}^{n} \binom{n}{r} \frac{x^{-\sigma_0+\alpha(n-r)}}{f(x)} t_{n-r}(x) \, x^{\alpha+1+\alpha(r-1)} f(x) s_{r-1}(x)}{\frac{x^{-\sigma_0+\alpha\, n}}{f(x)} t_n(x)} \\
&= x\, f(x) \frac{\sum_{r=1}^{n} \binom{n}{r} \, t_{n-r}(x) \, s_{r-1}(x)}{t_n(x)} \\
&= x\, f(x) \frac{a_n(x)}{b_n(x)}, \qquad (5.26)
\end{aligned}$$

where the polynomials $a_n(x)$ and $b_n(x)$ and the bounds on their degrees are as prescribed above. $\square$

Before applying these tools to the five examples above, we take a moment to discuss a special class of rational approximants, the Padé approximants [67]. Consider the (formal) power series $\mathcal{F}(x) = \sum_{i=0}^{\infty} f_i x^i$ as $x \to 0$. Then the Padé approximants $[l/m]_f(x)$ to $\mathcal{F}(x)$ are the rational approximants:

$$\frac{P^{[l/m]}(x)}{Q^{[l/m]}(x)} = \frac{p_0 + p_1 x + \cdots + p_l x^l}{q_0 + q_1 x + \cdots + q_m x^m} \qquad \text{with} \qquad l, m \in \mathbb{N}_0, \qquad (5.27)$$

which satisfy the maximal accuracy-through-order condition:

$$\mathcal{F}(x) - \frac{P^{[l/m]}(x)}{Q^{[l/m]}(x)} = \mathcal{O}(x^{l+m+1}), \quad \text{as} \quad x \to 0. \qquad (5.28)$$

Of course, this formalism for the construction of Padé approximants also works if we start from an inverse power series. The only difference is that we then obtain Padé approximants in $1/x$ instead of x. This modified asymptotic condition is then:

$$\mathcal{F}(1/x) - \frac{P^{[l/m]}(1/x)}{Q^{[l/m]}(1/x)} = \mathcal{O}\left(\frac{1}{x^{l+m+1}}\right) \qquad \text{as} \qquad x \to \infty. \tag{5.29}$$

5.A.1 The distributions

In applying Theorems 5.1 and 5.2, we first consider the standard normal distribution, where:

$$g_N(x) = A\, x^{\mu} e^{r(x)}, \tag{5.30}$$

where $A^{-1} = \sqrt{2\,\pi}$, $\mu = 0$ and $r(x) = -x^2/2$. The approximations take the form:

$$\tilde{G}_n^{(1)}(x) = x\, g_N(x) \frac{a_n(x)}{b_n(x)}, \tag{5.31}$$

where $\deg(a_n(x)) \leq 2n - 2$ and $\deg(b_n(x)) = 2n$, which is in agreement with (4.28). The approximations $\tilde{G}_n^{(1)}(x) = \tilde{G}_n^{(1,1)}(x)$ satisfy the asymptotic error estimate:

$$\frac{\tilde{G}_n^{(1)}(x)}{g_N(x)/x} - \frac{\int_x^{\infty} g_N(t)\, \mathrm{d}t}{g_N(x)/x} = \mathcal{O}\left(\frac{1}{x^{3n}}\right) \quad \text{as} \quad x \to \infty. \tag{5.32}$$

The case for the general normal distribution $f_N(x)$ may be developed similarly.

We next consider the gamma distribution, where:

$$f_g(x) = A\, x^{\mu} e^{r(x)}, \tag{5.33}$$

where $A^{-1} = \Gamma(a)\, b^a$, $\mu = a - 1$ and $r(x) = -x/b$. The approximations, then, take the form:

$$\tilde{G}_n^{(1)}(x) = x\, f_g(x) \frac{a_n(x)}{b_n(x)}, \tag{5.34}$$

where $\deg(a_n(x)) \leq n-1$ and $\deg(b_n(x)) = n$, which is in agreement with (4.34). The approximations $\tilde{G}_n^{(1)}(x) = \tilde{G}_n^{(1,1)}(x)$ satisfy the asymptotic error estimate:

$$\frac{\tilde{G}_n^{(1)}(x)}{f_g(x)} - \frac{\int_x^\infty f_g(t)\,\mathrm{d}t}{f_g(x)} = \mathcal{O}\left(\frac{1}{x^{2n}}\right) \quad \text{as} \quad x \to \infty. \tag{5.35}$$

In fact, given the accuracy-through-order condition derived above, the bound on the degree of $a_n(x)$ can be made more precise. Indeed, $\deg(a_n(x)) = n-1$. Furthermore, the rational approximants of (4.34) are Padé approximants in inverse powers of x as $x \to \infty$.

We consider the student's t-distribution. In this case, only the asymptotic error estimate for the approximations $\tilde{G}_n^{(1)}(x) = \tilde{G}_n^{(1,1)}(x)$ can be deduced, as Theorem 5.2 does not apply. Since $\omega(x) = x\,f_t(x)$, the approximations satify:

$$\frac{\tilde{G}_n^{(1)}(x)}{x\,f_t(x)} - \frac{\int_x^\infty f_t(t)\,\mathrm{d}t}{x\,f_t(x)} = \mathcal{O}\left(\frac{1}{x^{n}}\right) \quad \text{as} \quad x \to \infty. \tag{5.36}$$

We consider the inverse Gaussian distribution. In this case, only the asymptotic error estimate for the approximations $\tilde{G}_n^{(1)}(x) = \tilde{G}_n^{(1,1)}(x)$ can be deduced, as Theorem 5.2 does not apply. Since $\omega(x) = f_i(x)$, the approximations satify:

$$\frac{\tilde{G}_n^{(1)}(x)}{f_i(x)} - \frac{\int_x^\infty f_i(t)\,\mathrm{d}t}{f_i(x)} = \mathcal{O}\left(\frac{1}{x^{2n}}\right) \quad \text{as} \quad x \to \infty. \tag{5.37}$$

Lastly, we consider Fisher's F distribution. In this case, only the asymptotic error estimate for the approximations $\tilde{G}_n^{(1)}(x) = \tilde{G}_n^{(1,1)}(x)$ can be deduced, as Theorem 5.2 does not apply. Since $\omega(x) = x\,f_F(x)$, the approximations satify:

$$\frac{\tilde{G}_n^{(1)}(x)}{x\,f_F(x)} - \frac{\int_x^\infty f_F(t)\,\mathrm{d}t}{x\,f_F(x)} = \mathcal{O}\left(\frac{1}{x^{n}}\right) \quad \text{as} \quad x \to \infty. \tag{5.38}$$

Remark:

1. Theorem 2 in [13] provides the first accuracy-through-order condition for the $G_n^{(m)}$ transformation in the literature. It states that, among other conditions, if $F(x) \to I[f]$ as $x \to \infty$ then:

$$\frac{I[f] - G_n^{(m)}}{I[f] - F(x)} = \mathcal{O}\left(\frac{1}{x^n}\right) \quad \text{as} \quad x \to \infty. \tag{5.39}$$

   They prove this result explicitly for $m = 1$ using the determinantal formula derived from the system of equations (3.9). By using the algorithmic form for $G_n^{(1)}$ and its generalization $G_n^{(1,\alpha)}$, we are able to prove in Theorem 5.1 a different result, one which depends more closely on the integrand, specifically, $\deg(r(x)) = r_0$.

2. The asymptotic expansion suggested by equations (3.6) and (3.9), is the asymptotic expansion in (5.11) with $\omega(x) = x^{\sigma_0} f(x)$ and $\alpha = 1$. It is known that for $f(x) \in \mathbf{B}^{(1)}$, satisfying a first order linear homogeneous differential equation, this asymptotic expansion is certainly true and valid. However, it may be that different values of α exist which may lead to different approximations $G_n^{(1,\alpha)}$. For example, it is known that the asymptotic expansion of the tail integral of the standard normal distribution is more concisely given in inverse powers of x^2 as in:

$$\int_x^\infty \frac{e^{-t^2/2}}{\sqrt{2\,\pi}}\,\mathrm{d}t \sim \frac{e^{-x^2/2}}{x\sqrt{2\,\pi}} \sum_{i=0}^\infty \frac{(-2)^i (1/2)_i}{x^{2\,i}}, \quad \text{as} \quad x \to \infty, \tag{5.40}$$

   than simply in inverse powers of x. In cases like these, where such an $\alpha \neq 1$ can be legitimately found, then the $G_n^{(1,\alpha)}$ transformation may be applied to obtain a higher accuracy-through-order condition than that obtained through $G_n^{(1)}$. However, in approximating the value of a tail integral as $x \to 0$, or even for a medium-valued x, a higher accuracy-through-order condition may not help, as there are other factors which govern convergence.

3. Theorem 5.2 does not apply to the approximations of the student's t, Fisher's F and the inverse Gaussian distributions. Other general forms for integrands such as $f(x) = x^\mu \frac{p(x)}{q(x)}$ or even $f(x) = x^\mu \frac{p(x)}{q(x)} \exp(x^\nu r(x))$ where $\mu \in \mathbb{R}$, $\nu \in \mathbb{Z}$, $p(x) \in \mathbb{R}[x]$, $q(x) \in \mathbb{R}[x]$ and $r(x) \in \mathbb{R}[x]$ may be able to provide further insight in the forms of rational approximants derived from the G transformation; however, the introduction of a rational function dramatically increases the upper bounds to the degrees in the polynomials in the analogous Lemma 5.1 (by the quotient rule for derivatives) such that they are neither accurate nor helpful in characterizing the overall solution.

5.B Correspondence with continued fractions

In this section, we search for a different method of computing the $\tilde{G}_n^{(1)}(x)$ transformation, as the ratio of polynomials is neither recursive nor stable as $n \to \infty$. The method of Viskovatov [68] allows for the transformation of a ratio of infinite series to a continued fraction. Before we present the method, and its modifications to explicitly demonstrate the correspondence as $x \to \infty$ in our case, we begin with some preliminaries on continued fractions. A continued fraction [69] is an expression of the form:

$$b_0 + \cfrac{a_1}{b_1 + \cfrac{a_2}{b_2 + \cfrac{a_3}{b_3 + \ddots}}} \tag{5.41}$$

where the sequences $\{a_m\}_{m=1}^{\infty}$ and $\{b_m\}_{m=1}^{\infty}$ are, in general, sequences of complex numbers. Recently, more effective notation has been introduced to alleviate the descending staircase aspect of continued fractions. Equation (5.41) may be represented by:

$$b_0 + \frac{a_1}{b_1 +} \frac{a_2}{b_2 +} \frac{a_3}{b_3 +} \cdots \quad \text{or} \tag{5.42}$$

$$b_0 + \mathop{\mathrm{K}}_{m=1}^{\infty} \left(\frac{a_m}{b_m} \right). \tag{5.43}$$

The symbol K in the (infinite) continued fraction (5.43) comes from the German *Kettenbruch*, and is the analogue of the symbol Σ in (infinite) summations. In addition, the n^{th} approximant is denoted by the complex number:

$$f_n = b_0 + \cfrac{a_1}{b_1 + \cfrac{a_2}{b_2 + \cfrac{a_3}{b_3 + \ddots + \cfrac{a_n}{b_n}}}} \tag{5.44}$$

or:

$$f_n = b_0 + \frac{a_1}{b_1} \mathop{+}\limits \frac{a_2}{b_2} \mathop{+}\limits \frac{a_3}{b_3} + \cdots + \frac{a_n}{b_n} \quad \text{or} \tag{5.45}$$

$$f_n = b_0 + \mathop{\mathrm{K}}_{m=1}^{n} \left(\frac{a_m}{b_m} \right). \tag{5.46}$$

5.B.1 S-fractions and their convergence

A continued fraction of the form:

$$F(z) = \mathop{\mathrm{K}}_{m=1}^{\infty} \left(\frac{a_m z}{1} \right), \qquad a_m > 0, \tag{5.47}$$

is called a Stieltjes fraction or *S-fraction*.

A convergence result for S-fractions

Theorem 5.3 ([69]): *An S-fraction* $\mathrm{K}(a_m z/1)$ *corresponding at* $z = 0$ *to* $L(z) = \sum_{k=1}^{\infty} c_k z^k$ *is convergent in* $\{z \in \mathbb{C} : |\arg z| < \pi\}$ *if one of the following conditions holds:*

1.

$$a_m \leq M, \qquad m = 1, 2, \ldots, \tag{5.48}$$

2.

$$\sum_{m=1}^{\infty} \frac{1}{\sqrt{a_m}} = \infty, \tag{5.49}$$

3. Carleman criterion:

$$\sum_{k=1}^{\infty} \frac{1}{|c_k|^{\frac{1}{2k}}} = \infty. \tag{5.50}$$

If the S-fraction $\mathrm{K}(a_m z/1)$ *is convergent, then it converges to a finite value.*

5.B.2 The modified method of Viskovatov

Let $\{c_{0,i}\}$ and $\{c_{1,i}\}$ be sequences in $\mathbb{C}$ and for $x \in \mathbb{C}/0$, consider the quotient:

$$\frac{\sum_{i=0}^{\infty} c_{1,i} x^{-i}}{\sum_{i=0}^{\infty} c_{0,i} x^{-i}}. \tag{5.51}$$

This may be rewritten as:

$$\frac{1}{\frac{c_{0,0}}{c_{1,0}} + \frac{\sum_{i=0}^{\infty} c_{0,i} x^{-i}}{\sum_{i=0}^{\infty} c_{1,i} x^{-i}} - \frac{c_{0,0}}{c_{1,0}}}, \tag{5.52}$$

$$= \frac{1}{\frac{c_{0,0}}{c_{1,0}} + \frac{c_{1,0}\sum_{i=0}^{\infty} c_{0,i} x^{-i} - c_{0,0}\sum_{i=0}^{\infty} c_{1,i} x^{-i}}{c_{1,0}\sum_{i=0}^{\infty} c_{1,i} x^{-i}}}, \tag{5.53}$$

$$= \frac{\frac{c_{1,0}}{c_{0,0}}}{1 + \frac{\sum_{i=0}^{\infty} \left(\frac{c_{1,0}c_{0,i} - c_{0,0}c_{1,i}}{c_{0,0}} \right) x^{-i}}{\sum_{i=0}^{\infty} c_{1,i} x^{-i}}}, \tag{5.54}$$

$$= \frac{\frac{c_{1,0}}{c_{0,0}}}{1 + \frac{\frac{1}{x}\sum_{i=0}^{\infty} c_{2,i} x^{-i}}{\sum_{i=0}^{\infty} c_{1,i} x^{-i}}}, \tag{5.55}$$

where:

$$c_{2,i} := \frac{c_{1,0}c_{0,i+1} - c_{0,0}c_{1,i+1}}{c_{0,0}} \quad \forall i \in \mathbb{N}_0. \tag{5.56}$$

Notice, now, that in the bottom right corner of (5.55), there is another ratio of asymptotic expansions and compared with (5.51), the first indices on the coefficients $c_{k,i}$ is increased by 1. Applying this technique recursively, we are able to transform a ratio of asymptotic expansions into a modified S-fraction [69].

The modified method of Viskovatov

Let $\{c_{0,i}\}$ and $\{c_{1,i}\}$ be sequences in $\mathbb{C}$ and for $x \in \mathbb{C}/0$, consider the quotient (5.51). Define the sequences:

$$c_{k,i} := \frac{c_{k-1,0}c_{k-2,i+1} - c_{k-2,0}c_{k-1,i+1}}{c_{k-2,0}}, \qquad k \geq 2, \quad i = 0, 1, \ldots. \tag{5.57}$$

The quotient (5.51) may be written as the continued fraction:

$$x \mathop{\mathrm{K}}_{m=1}^{\infty} \left(\frac{(c_{m,0}/c_{m-1,0})/x}{1} \right). \tag{5.58}$$

Naturally, if for some integers M and N the terms in the sequences $c_{0,i} = 0$, $i > M$ and $c_{1,i} = 0$, $i > N$, then the continued fraction (5.58) should be truncated after the P^{th} approximant, $P = \max\{M, N\}$.

5.B.3 Correspondence with continued fractions

With the necessary preliminaries given on continued fractions, we establish the correspondence of continued fractions of the form (5.58) with the Padé-type approximants developed for the $\tilde{G}_n^{(1)}$ transformation.

Theorem 5.4: *Let $f(x)$ be a function of the form prescribed in Theorem 5.2. Let $M = n\,r_0$ and let $N = (n-1)r_0$ such that $P = \max\{M, N\} = M$. Furthermore, let the approximants (5.23) be written as:*

$$\frac{\tilde{G}_n^{(1)}(x)}{x\,f(x)} = \frac{a_n(x)}{b_n(x)}, \tag{5.59}$$

$$= x^{-r_0} \frac{\sum_{i=0}^{N} a_{N-i}^{(n)} x^{-i}}{\sum_{i=0}^{M} b_{M-i}^{(n)} x^{-i}}, \tag{5.60}$$

where the superscript $^{(n)}$ *on the coefficients respects the order* n *of the* $\tilde{G}_n^{(1)}$ *transformation. Define the sequences:*

$$c_{0,i}^{(n)} := b_{M-i}^{(n)}, \quad i = 0, 1, \ldots, M, \tag{5.61}$$

$$c_{1,i}^{(n)} := a_{N-i}^{(n)}, \quad i = 0, 1, \ldots, N, \qquad c_{1,i}^{(n)} := 0, \quad i = N+1, \ldots, M, \tag{5.62}$$

$$c_{k,i}^{(n)} := \frac{c_{k-1,0}^{(n)} c_{k-2,i+1}^{(n)} - c_{k-2,0}^{(n)} c_{k-1,i+1}^{(n)}}{c_{k-2,0}^{(n)}}, \qquad k \geq 2, \quad i = 0, 1, \ldots, M-k. \tag{5.63}$$

Then the approximants (5.23) *may be written as:*

$$\frac{\tilde{G}_n^{(1)}(x)}{x\, f(x)} = x^{1-r_0} \mathop{\mathrm{K}}_{m=1}^{M} \left(\frac{(c_{m,0}^{(n)}/c_{m-1,0}^{(n)})/x}{1} \right). \tag{5.64}$$

Proof. With the approximants written explicitly as in (5.60), and the sequences defined as in (5.61)–(5.63), the modified method of Viskovatov may be applied to transform the quotient of (5.60) into a continued fraction. □

Theorem 5.5: *Let* $f(x)$ *be a function of the form prescribed in Theorem 5.2. Let the approximants:*

$$\frac{\tilde{G}_n^{(1)}(x)}{x\, f(x)} \tag{5.65}$$

be written as the continued fraction (5.64)*. The sequence of continued fractions* (5.64) *corresponds to the formal power series of:*

$$\frac{\int_x^\infty f(t)\,\mathrm{d}t}{x\, f(x)} = \sum_{i=0}^{\infty} \frac{\beta_{0,i}}{x^i}, \qquad \text{at} \quad x = \infty. \tag{5.66}$$

Proof. By equality in (5.64), the asymptotic condition (5.22) holds for the continued fraction $\forall n \in \mathbb{N}$. □

5.C Extrapolation to the limit

With the $\tilde{G}_n^{(1)}$ transformation defined by the ratio in (5.23), and with knowledge of the large asymptotic growth of specific examples of the coefficients of those polynomials[1] it becomes difficult to answer the question:

$$\text{What is } \lim_{n\to\infty} \tilde{G}_n^{(1)}(x) \text{ ?} \tag{5.67}$$

With the material developed in the preceding section on the correspondence with continued fractions, we are now capable of addressing the question with a more convenient approach. In this section, we intend to develop the continued fractions for the approximations $\tilde{G}_n^{(1)}(x)$ for the tail integrals of the normal distribution and the gamma distribution. As continued fractions, we examine their convergence.

[1]This comes from equations (4.28) and (4.34) and from the asymptotics of the A_k^i derived in subsection 2.B.2.

5.C.1 The normal distribution

From (4.28), we use simple algebraic manipulations to render the approximations to the form:

$$\frac{\tilde{G}_n^{(1)}(z)}{z\,g_N(z)} = \frac{1}{z^2}\left[\frac{\displaystyle\sum_{i=0}^{n-1}\left\{\sum_{r=1}^{n}\binom{n}{r}\left(\sum_{l=0}^{n-1-i}(-1)^l A_{n-r}^{n-1-i-l}B_{r-1}^{l}\right)\right\}z^{-2i}}{\displaystyle\sum_{i=0}^{n}A_n^{n-i}z^{-2i}}\right], \tag{5.68}$$

$$= \frac{1}{x}\frac{\displaystyle\sum_{i=0}^{n-1}c_{1,i}^{(n)}x^{-i}}{\displaystyle\sum_{i=0}^{n}c_{0,i}^{(n)}x^{-i}}, \tag{5.69}$$

where:

$$x := z^2, \qquad c_{0,i}^{(n)} := A_n^{n-i}, \tag{5.70}$$

$$c_{1,i}^{(n)} := \sum_{r=1}^{n}\binom{n}{r}\left(\sum_{l=0}^{n-1-i}(-1)^l A_{n-r}^{n-1-i-l}B_{r-1}^{l}\right). \tag{5.71}$$

Then, from the sequences (5.61)–(5.63), we obtain the continued fraction:

$$\frac{\tilde{G}_n^{(1)}(z)}{z\,g_N(z)} = \operatorname*{K}_{m=1}^{n}\left(\frac{(c_{m,0}^{(n)}/c_{m-1,0}^{(n)})/z^2}{1}\right), \tag{5.72}$$

and in the limiting case, the sequence $\{c_{m,0}^{(n)}\}_{m=0}^{\infty}$ as $n \to \infty$ is of interest. Numerical computations with symbolic software help reveal that $c_{0,0}^{(n)} = 1$, $c_{1,0}^{(n)} = 1$, $c_{2,0}^{(n)} = 1$, $c_{3,0}^{(n)} = 2$, $c_{4,0}^{(n)} = 6, \ldots, \forall n \in \mathbb{N}$. At this point in time, we conjecture that $c_{m,0} = (m-1)!$ for $m > 0$, and so:

$$\lim_{n\to\infty} \tilde{G}_n^{(1)}(z) = z\, g_N(z) \left(\frac{1}{z^2 + \underset{m=1}{\overset{\infty}{\mathrm{K}}} \left(\frac{m/z^2}{1} \right)} \right), \tag{5.73}$$

a convergent S-fraction result that is, after an equivalence transformation, given in [69].

5.C.2 The gamma distribution

From (4.34), we use simple algebraic manipulations to render the approximations to the form:

$$\frac{\tilde{G}_n^{(1)}(x)}{x\, f_g(x)} = \frac{b}{x} \left[\frac{\displaystyle\sum_{i=0}^{n-1} \left\{ \sum_{r=1}^{n} \binom{n}{r} \left(\sum_{l=0}^{n-1-i} (-1)^l A_{n-r}^{n-1-i-l} B_{r-1}^{l} \right) \right\} \left(\frac{x}{b}\right)^{-i}}{\displaystyle\sum_{i=0}^{n} A_n^{n-i} \left(\frac{x}{b}\right)^{-i}} \right], \tag{5.74}$$

$$= \frac{1}{\xi} \frac{\displaystyle\sum_{i=0}^{n-1} c_{1,i}^{(n)} \xi^{-i}}{\displaystyle\sum_{i=0}^{n} c_{0,i}^{(n)} \xi^{-i}}, \tag{5.75}$$

where:

$$\xi := \frac{x}{b}, \qquad c_{0,i}^{(n)} := A_n^{n-i}, \tag{5.76}$$

$$c_{1,i}^{(n)} := \sum_{r=1}^{n} \binom{n}{r} \left(\sum_{l=0}^{n-1-i} (-1)^l A_{n-r}^{n-1-i-l} B_{r-1}^{l} \right). \tag{5.77}$$

Then, from the sequences (5.61)–(5.63), we obtain the continued fraction:

$$\frac{\tilde{G}_n^{(1)}(x)}{x\, f_g(x)} = \underset{m=1}{\overset{n}{\mathrm{K}}} \left(\frac{(c_{m,0}^{(n)}/c_{m-1,0}^{(n)})\, b/x}{1} \right), \tag{5.78}$$

and in the limiting case, the sequence $\{c_{m,0}^{(n)}\}_{m=0}^{\infty}$ as $n \to \infty$ is of interest. Numerical computations with symbolic software help reveal that $c_{0,0}^{(n)} = 1$, $c_{1,0}^{(n)} = 1$, $c_{2,0}^{(n)} = 1 - a$, $c_{3,0}^{(n)} = 1 - a$, $c_{4,0}^{(n)} = (2-a)(1-a), \ldots, \forall n \in \mathbb{N}$. At this point in time, we conjecture that:

$$\lim_{n\to\infty} \tilde{G}_n^{(1)}(x) = x\, f_g(x) \mathop{\mathrm{K}}_{m=1}^{\infty} \left(\frac{a_m(a)\, b/x}{1} \right), \tag{5.79}$$

where:

$$a_1(a) = 1, \quad a_{2j}(a) = j - a, \quad a_{2j+1}(a) = j, \quad j \geq 1. \tag{5.80}$$

This convergent S-fraction result is given in [69].

Chapter 6

Conclusion

This thesis is concerned with the development of new formulae for higher order derivatives, and the algorithmic, numerical, and analytical development of the $G_n^{(1)}$ transformation, a method for computing infinite-range integrals. We introduce the Slevinsky-Safouhi formulae I and II with applications, we develop an algorithm for the $G_n^{(1)}$ transformation, we derive explicit approximations to incomplete Bessel functions and tail probabilities of five probability distributions from the recursive algorithm for the $G_n^{(1)}(x)$ transformation, and we present all extant work on the analysis of the convergence properties of the $G_n^{(1)}$ transformation.

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