



New formulae for higher order derivatives and applications

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ABSTRACT

We present new formulae (the Slevinsky–Safouhi formulae I and II) 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. We also presented an application of the formulae of higher order derivatives combined with extrapolation methods in the numerical integration of spherical Bessel integral functions.

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1. Introduction

In the present work, we present new analytic formulae (the Slevinsky–Safouhi formulae I and II) that allow for the calculation of higher order derivatives. These formulae are applicable to functions $G(x)$ for which the terms $\left(\frac{d}{x^m dx}\right)^k (x^{-n} G(x))$ for some m, n are well-defined. 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 $\frac{d^{14}}{dx^{14}} j_n(vx) \Big|_{(n,v,x)=(1,1,1)}$ 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.

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 [1] and the challenging spherical Bessel integrals involved in the so-called molecular integrals over exponential type functions [2–4] and in integrals of magnetic properties of molecules [5]. The nonlinear D and G transformations [6,7] have proven to be very powerful tools in the computation of molecular integrals [8–13] and the Twisted Tail [14]. Moreover, the algorithms of these transformations require successive derivatives of the integrands, which can be a severe computational impediment. In the case of the G transformation, higher order derivatives of the integrands are required for the calculation. In highly oscillatory integrands, special functions, like spherical and reduced Bessel functions are prevalent.

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As the radial solution of the Helmholtz equation, and as functions satisfying Sturm–Liouville boundary value problems, Bessel functions have grown to become very prominent special functions in mathematics and science. Applications include the Mie solution to Maxwell's equations for the scattering of electromagnetic waves off spherical particles [15], the solution of the Schrödinger equation subjected to an infinite spherical well potential, modeling a quantum dot [16] and other applications in quantum chemistry due to Rayleigh's plane wavefunction expansion [17]. Bessel functions are exceptionally difficult functions to compute; that recurrence relations are only stable in certain directions and that cylindrical Bessel functions (of integral order) do not have simple analytical expressions are among the many reasons why they pose as great numerical problems.

As examples of applications, we develop higher order derivatives of Legendre functions, Chebyshev polynomials of the first kind, Hermite functions and Bessel functions. For all of these examples, we also perform numerical computations and provide tables illustrating our results herein. We also present an efficient algorithm obtained from the Slevinsky–Safouhi formula I for the numerical integration of highly oscillatory spherical Bessel integrals, which are involved in molecular structure calculations and are known to be extremely difficult to evaluate rapidly to a high pre-determined accuracy. In addition, we show the most general cases of our formula, notably, $\frac{d^k}{dx^k}(x^n f(x^{m+1}))$, $\frac{d^k}{dx^k}(x^n f(\ln(x)))$ and $\frac{d^k}{dx^k}(e^{nx} f(e^x))$. We also develop a new method based on our formulae for solving and/or characterizing certain classes of differential equations.

2. 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 [18] for other differentiation formulae.

Formula 2.1 (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:

$$f^{(k)}(x) = \sum_{n=0}^k \binom{k}{n} g^{(n)}(x) h^{(k-n)}(x), \quad (1)$$

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 2.2 (The Quotient Formula). For a function $f(x) = \frac{g(x)}{h(x)}$, 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:

$$f^{(k)}(x) = \frac{g^{(k)}(x) - \sum_{n=0}^{k-1} \binom{k}{n} f^{(n)}(x) h^{(k-n)}(x)}{h(x)}. \quad (2)$$

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 2.3 (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:

$$f^{(m+n)}(x) = \sum_{k=0}^{m-1} \sum_{i=0}^n \binom{n}{i} p_k^{(i)}(x) f^{(k+n-i)}(x), \quad (3)$$

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

Formula 2.4 (Faà di Bruno's Formula [19–21]). For a function $f(g(x))$:

$$\frac{d^n}{dx^n} f(g(x)) = \sum n! f^{(k)}(g(x)) \prod_{i=1}^n \frac{1}{k_i!} \left(\frac{g^{(i)}(x)}{i!} \right)^{k_i}, \quad (4)$$

where the summation is over all non-negative integer solutions of the Diophantine equation (5) and where k is the count of all non-zero k_i 's involved in:

$$\sum_{i=1}^n i k_i = n. \quad (5)$$

3. New formula for higher order derivatives

Theorem 3.1 (The Slevinsky–Safouhi Formula I). Let $G(x)$ be a function k th differentiable and with the term $\left(\frac{d}{x^\mu dx}\right)^k (x^{-n}G(x))$ well-defined. The term $\left(\frac{d}{x^\mu dx}\right)^k (x^{-\nu}G(x))$ is given by:

$$\left(\frac{d}{x^\mu dx}\right)^k (x^{-\nu}G(x)) = \sum_{i=0}^k A_k^i x^{n-\nu+i(m+1)-k(\mu+1)} \left(\frac{d}{x^m dx}\right)^i (x^{-n}G(x)), \quad (6)$$

with coefficients:

$$A_k^i = \begin{cases} 1 & \text{for } i = k, \\ (n - \nu - (k - 1)(\mu + 1))A_{k-1}^0 & \text{for } i = 0, k > 0, \\ (n - \nu + i(m + 1) - (k - 1)(\mu + 1))A_{k-1}^i + A_{k-1}^{i-1} & \text{for } 0 < i < k. \end{cases} \quad (7)$$

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

$$A_k^i = \sum_{j=0}^i \frac{(-1)^{i-j} (n - \nu + j(m + 1) - (k - 1)(\mu + 1))_{k, \mu+1}}{(m + 1)^j j! (i - j)!}, \quad (8)$$

where $(x)_{n,k}$ is the Pochhammer k -symbol [22] and can be computed as $\prod_{l=0}^{k-1} (x + kl)$.

Proof of Theorem 3.1. It is easy to show that Eq. (6) holds for $k = 0$, since:

$$x^{-\nu}G(x) = x^{n-\nu}(x^{-n}G(x)). \quad (9)$$

For $k = 1$, we show that Eqs. (6) and (7) hold by applying $\left(\frac{d}{x^\mu dx}\right)$ to both sides of (9):

$$\left(\frac{d}{x^\mu dx}\right) (x^{-\nu}G(x)) = (n - \nu)x^{n-\nu-\mu-1}(x^{-n}G(x)) + x^{n-\nu+m-\mu} \left(\frac{d}{x^m dx}\right) (x^{-n}G(x)). \quad (10)$$

As (6) and (7) are true for $k = 0, 1$, we now assume they hold for $k - 1$:

$$\left(\frac{d}{x^\mu dx}\right)^{k-1} (x^{-\nu}G(x)) = \sum_{i=0}^{k-1} A_{k-1}^i x^{n-\nu+i(m+1)-(k-1)(\mu+1)} \left(\frac{d}{x^m dx}\right)^i (x^{-n}G(x)). \quad (11)$$

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

$$\begin{aligned} \left(\frac{d}{x^\mu dx}\right)^k (x^{-\nu}G(x)) &= \frac{d}{x^\mu dx} \sum_{i=0}^{k-1} A_{k-1}^i x^{n-\nu+i(m+1)-(k-1)(\mu+1)} \left(\frac{d}{x^m dx}\right)^i (x^{-n}G(x)) \\ &= \sum_{i=0}^{k-1} A_{k-1}^i \left[(n - \nu + i(m + 1) - (k - 1)(\mu + 1))x^{n-\nu+i(m+1)-k(\mu+1)} \left(\frac{d}{x^m dx}\right)^i (x^{-n}G(x)) \right. \\ &\quad \left. + x^{n-\nu+(i+1)(m+1)-k(\mu+1)} \left(\frac{d}{x^m dx}\right)^{i+1} (x^{-n}G(x)) \right]. \end{aligned} \quad (12)$$

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

$$\left(\frac{d}{x^\mu dx}\right)^k (x^{-\nu}G(x)) = (n - \nu - (k - 1)(\mu + 1))A_{k-1}^0 x^{n-\nu-k(\mu+1)} (x^{-n}G(x)) \quad (13)$$

$$\begin{aligned} &+ \sum_{i=1}^{k-1} [(n - \nu + i(m + 1) - (k - 1)(\mu + 1))A_{k-1}^i + A_{k-1}^{i-1}] x^{n-\nu+i(m+1)-k(\mu+1)} \left(\frac{d}{x^m dx}\right)^i (x^{-n}G(x)) \\ &+ A_{k-1}^{k-1} x^{n-\nu+k(m-\mu)} \left(\frac{d}{x^m dx}\right)^k (x^{-n}G(x)), \end{aligned} \quad (14)$$

which recovers the recurrence relations for the coefficients in (7).

To prove the explicit expression (8), consider the main recurrence relation:

$$A_k^i = (n - \nu + i(m + 1) - (k - 1)(\mu + 1))A_{k-1}^i + A_{k-1}^{i-1}, \quad (15)$$

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

We begin by defining the auxiliary coefficients:

$$D_k^i = (n - \nu + i(m + 1) - (k - 1)(\mu + 1))D_{k-1}^i \quad \text{and} \quad D_0^i = 1, \quad (16)$$

that have the simple explicit solution:

$$D_k^i = (n - \nu + i(m + 1) - (k - 1)(\mu + 1))_{k, \mu+1}. \quad (17)$$

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

$$\begin{cases} D_k^1 = (m + 1)A_k^1 + A_k^0 = (m + 1)A_k^1 + D_k^0 \\ D_k^2 = 2(m + 1)^2A_k^2 + 2(m + 1)A_k^1 + A_k^0 = 2(m + 1)^2A_k^2 + 2D_k^1 - D_k^0, \end{cases} \quad (18)$$

and in general:

$$D_k^i = i!(m + 1)^i A_k^i + \sum_{j=0}^{i-1} \binom{i}{j} (-1)^{i-1-j} D_k^j, \quad (19)$$

which ultimately leads to:

$$A_k^i = \sum_{j=0}^i \frac{(-1)^{i-j} D_k^j}{(m + 1)^j j! (i - j)!}, \quad (20)$$

whereupon the explicit expression for the coefficients is easily deduced. For $m = -1$, we note that $D_k^0 = D_k^1 = \dots = D_k^k$. 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 3.2 (The Slevinsky–Safouhi Formula II). Let $G(x)$ be a function k th differentiable and with the term $\left(\frac{d}{xdx}\right)^k G(x)$ well-defined. The term $\frac{d^k G}{dx^k}$ is given by:

$$\frac{d^k G}{dx^k} = \sum_{i=\lfloor \frac{k+1}{2} \rfloor}^k \hat{A}_k^i x^{2i-k} \left(\frac{d}{xdx}\right)^i G(x), \quad (21)$$

with coefficients:

$$\hat{A}_k^i = \begin{cases} 1 & \text{for } i = k \\ 2\hat{A}_{k-1}^i + \hat{A}_{k-1}^{i-1} & \text{for } i = \left\lfloor \frac{k+1}{2} \right\rfloor, k \text{ odd} \\ \hat{A}_{k-1}^i & \text{for } i = \left\lfloor \frac{k+1}{2} \right\rfloor, k \text{ even} \\ (2i - k + 1)\hat{A}_{k-1}^i + \hat{A}_{k-1}^{i-1} & \text{for } \left\lfloor \frac{k+1}{2} \right\rfloor < i < k, k > 3, \end{cases} \quad (22)$$

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

Moreover, these coefficients have the explicit expression:

$$\hat{A}_k^i = \sum_{j=0}^i \frac{(-1)^{i-j} (2j - k + 1)_k}{2^j j! (i - j)!}, \quad (23)$$

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

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 point of view, recurrence relations are more efficient when evaluating a sequence of derivatives.

3.1. The generality

With no loss of generality, [Theorem 3.1](#) 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:

$$\left(\frac{d}{x^m dx}\right)^i (x^{-n} G(x)) = \left(\frac{d}{x^m dx}\right)^i f(x^{m+1}) = (m+1)^i f^{(i)}(x^{m+1}), \quad (24)$$

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

$$\frac{d^k}{dx^k} (x^n f(x^{m+1})) = \sum_{i=0}^k A_k^i x^{n+i(m+1)-k} (m+1)^i f^{(i)}(x^{m+1}), \quad (25)$$

with coefficients A_k^i given by [\(7\)](#). Higher order derivatives of $f(x^{m+1})$ are developed in [\[18\]](#), and we present the formula here for comparison with [\(25\)](#):

$$\frac{d^k}{dx^k} f(x^{m+1}) = \sum_{i=0}^k \sum_{j=0}^i \frac{(-1)^j ((m+1)(i-j) - k + 1)_k f^{(i)}(x^{m+1})}{j!(i-j)! x^{k-i(m+1)}}. \quad (26)$$

Eqs. [\(25\)](#) and [\(26\)](#) are very similar in form and it is easy to show that [\(26\)](#) is a specific case of [Theorem 3.1](#). Note that the case $m = -1$ in [\(25\)](#) 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:

$$\left(x \frac{d}{dx}\right)^i (x^{-n} G(x)) = \left(x \frac{d}{dx}\right)^i f(\ln(x)) = f^{(i)}(\ln(x)), \quad (27)$$

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

$$\frac{d^k}{dx^k} (x^n f(\ln(x))) = \sum_{i=0}^k A_k^i x^{n-k} f^{(i)}(\ln(x)), \quad (28)$$

with coefficients A_k^i given by [\(7\)](#).

It is worth noting that higher order derivatives of $f(\ln(x))$ are given in [\[23\]](#) as:

$$\frac{d^k}{dx^k} f(\ln(x)) = \frac{1}{x^k} \sum_{i=1}^k (-1)^{k-i} \left[\begin{matrix} k \\ i \end{matrix} \right] f^{(i)}(\ln(x)), \quad (29)$$

where $\left[\begin{matrix} k \\ i \end{matrix} \right]$ are the Stirling numbers of the first kind. Thus formula [\(28\)](#) follows at once from [\(29\)](#) and the Leibniz formula.

Lastly, by performing the substitution $x \leftrightarrow e^x$ in [\(6\)](#) with $(\mu, \nu, m, n) = (-1, 0, 0, n)$, we obtain for the functions $G(x) = e^{nx} f(e^x)$:

$$\frac{d^k}{dx^k} (e^{nx} f(e^x)) = \sum_{i=0}^k A_k^i e^{(n+i)x} f^{(i)}(e^x), \quad (30)$$

with coefficients A_k^i given by [\(7\)](#), which again follows at once from:

$$\frac{d^k}{dx^k} f(e^x) = \sum_{i=1}^k \left\{ \begin{matrix} k \\ i \end{matrix} \right\} e^{ix} f^{(i)}(e^x), \quad (31)$$

found in [\[23\]](#) and the Leibniz formula. Here, $\left\{ \begin{matrix} k \\ i \end{matrix} \right\}$ 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 multiplied by $(-1)^{k-i}$ 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 3.1](#) and Faà di Bruno's formula ([Formula 2.4](#)) for $\frac{d^k}{dx^k} f(g(x))$, which has been recently applied in the numerical evaluation of a challenging integral [\[14\]](#). In approaching the general composition $f(g(x))$, we would naturally represent its derivatives as a linear combination of operators $\left(\frac{d}{g'(x)dx}\right)^k f(g(x)) = f^{(k)}(g(x))$. Indeed, the aforementioned representation forms the heart of Hoppe's Formula [\[21,24–26\]](#):

Formula 3.3 (Hoppe's Formula). For functions f and g sufficiently differentiable:

$$\frac{d^k}{dx^k} f(g(x)) = \sum_{i=0}^k \tilde{A}_k^i(x) f^{(i)}(g(x)), \quad (32)$$

where:

$$\tilde{A}_k^i(x) = \sum_{j=0}^i \frac{(-1)^{i-j}}{j!(i-j)!} (g(x))^{i-j} \frac{d^k}{dx^k} (g(x))^j. \quad (33)$$

It is mentioned in [21] that the functions $\tilde{A}_k^i(x)$ satisfy:

$$\tilde{A}_k^i(x) = \frac{d}{dx} \tilde{A}_{k-1}^i(x) + g'(x) \tilde{A}_{k-1}^{i-1}(x), \quad (34)$$

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 (33). With today's symbolic programming languages, Eq. (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 2.4).

3.2. Application to Legendre functions

The importance of higher order derivatives of Legendre functions is discussed in [27]. These aforementioned functions are defined through the Rodrigues formula [28]:

$$P_\ell^m(x) = \frac{(-1)^m}{2^\ell \ell!} (1-x^2)^{\frac{m}{2}} \frac{d^{\ell+m}}{dx^{\ell+m}} (x^2-1)^\ell. \quad (35)$$

Therefore, it is natural with the help of the Leibniz Formula (Formula 2.1) to define the higher order derivatives of these functions as:

$$\frac{d^k}{dx^k} P_\ell^m(x) = \frac{(-1)^m}{2^\ell \ell!} \sum_{n=0}^k \binom{k}{n} \frac{d^n}{dx^n} (1-x^2)^{\frac{m}{2}} \frac{d^{\ell+m+k-n}}{dx^{\ell+m+k-n}} (x^2-1)^\ell. \quad (36)$$

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

Considering that the identities:

$$\begin{cases} \left(\frac{d}{dx} \right)^i (1-x^2)^{\frac{m}{2}} = (-2)^i (1-x^2)^{\frac{m}{2}-i} \prod_{j=0}^{i-1} \left(\frac{m}{2} - j \right) \\ \left(\frac{d}{dx} \right)^i (x^2-1)^\ell = 2^i (x^2-1)^{\ell-i} \prod_{j=0}^{i-1} (\ell - j), \end{cases} \quad (37)$$

are computed with exceptional simplicity, we apply the result of Corollary 3.2 and develop:

$$\begin{cases} \frac{d^n}{dx^n} (1-x^2)^{\frac{m}{2}} = \sum_{i=\lfloor \frac{n+1}{2} \rfloor}^n \hat{A}_n^i x^{2i-n} (-2)^i (1-x^2)^{\frac{m}{2}-i} \prod_{j=0}^{i-1} \left(\frac{m}{2} - j \right) \\ \frac{d^{\ell+m+k-n}}{dx^{\ell+m+k-n}} (x^2-1)^\ell = \sum_{i=\lfloor \frac{\ell+m+k-n+1}{2} \rfloor}^{\ell+m+k-n} \hat{A}_{\ell+m+k-n}^i x^{2i-\ell-m-k+n} 2^i (x^2-1)^{\ell-i} \prod_{j=0}^{i-1} (\ell - j), \end{cases} \quad (38)$$

with coefficients $\hat{A}_k^i$ given by (22). This ultimately leads to the final result:

$$\begin{aligned} \frac{d^k}{dx^k} P_\ell^m(x) &= \frac{(-1)^m}{2^\ell \ell!} \sum_{n=0}^k \binom{k}{n} \left\{ \left[\sum_{i=\lfloor \frac{n+1}{2} \rfloor}^n \hat{A}_n^i x^{2i-n} (-2)^i (1-x^2)^{\frac{m}{2}-i} \prod_{j=0}^{i-1} \left(\frac{m}{2} - j \right) \right] \right. \\ &\quad \times \left. \left[\sum_{i=\lfloor \frac{\ell+m+k-n+1}{2} \rfloor}^{\ell+m+k-n} \hat{A}_{\ell+m+k-n}^i x^{2i-\ell-m-k+n} 2^i (x^2-1)^{\ell-i} \prod_{j=0}^{i-1} (\ell - j) \right] \right\}. \end{aligned} \quad (39)$$

Table 1Numerical evaluation of $\frac{d^k}{dx^k} P_\ell^m(x)$.

x	ℓ	m	k	Formula (39)	Values ^{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)

In [27], $\frac{d^k}{d\theta^k} P_\ell^m(\cos(\theta))$ is developed using recurrence relations as:

$$\frac{d^k}{d\theta^k} P_\ell^m(\cos(\theta)) = \frac{d^{k-1}}{d\theta^{k-1}} P_\ell^{m+1}(\cos(\theta)) - (\ell + m)(\ell - m + 1) \frac{d^{k-1}}{d\theta^{k-1}} P_\ell^{m-1}(\cos(\theta)), \quad (40)$$

and, for Legendre polynomials, there is [28]:

$$\frac{d^k}{dx^k} P_\ell(x) = \frac{d^{k-1}}{dx^{k-1}} P_{\ell-2}(x) + (2\ell - 1) \frac{d^{k-1}}{dx^{k-1}} P_{\ell-1}(x). \quad (41)$$

This simplicity cannot be extended to $\frac{d^k}{dx^k} P_\ell^m(x)$, as these recurrence relations have non-constant coefficients in x . There also exist a few large formulae for $\frac{d^k}{dx^k} P_\ell^m(x)$ in [29], some of which require hypergeometric series.

A Fortran program of (39) is created. A few sample calculations illustrating the method are included in Table 1. The results are compared to Maple 11's output with 18 correct digits in the evalf command.

3.3. Application to 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 [28]:

$$T_n(x) = \frac{\Gamma(\frac{1}{2})}{(-2)^n \Gamma(n + \frac{1}{2})} (1 - x^2)^{\frac{1}{2}} \frac{d^n}{dx^n} (1 - x^2)^{n - \frac{1}{2}}. \quad (42)$$

Therefore, it is natural with the help of the Leibniz Formula (Formula 2.1) to define the higher order derivatives of these functions as:

$$\frac{d^i}{dx^i} T_n(x) = \frac{\Gamma(\frac{1}{2})}{(-2)^n \Gamma(n + \frac{1}{2})} \sum_{l=0}^i \binom{i}{l} \frac{d^l}{dx^l} (1 - x^2)^{\frac{1}{2}} \frac{d^{n+i-l}}{dx^{n+i-l}} (1 - x^2)^{n - \frac{1}{2}}. \quad (43)$$

Without going into great detail, we regard this example as identical to the previous one. We apply the result of Corollary 3.2 and develop as the final result:

$$\begin{aligned} \frac{d^k}{dx^k} T_n(x) &= \frac{\Gamma(\frac{1}{2})}{(-2)^n \Gamma(n + \frac{1}{2})} \sum_{l=0}^k \binom{k}{l} \left\{ \left[\sum_{i=\lfloor \frac{l+1}{2} \rfloor}^l \hat{A}_i^l x^{2i-l} (-2)^i (1 - x^2)^{\frac{1}{2}-i} \prod_{j=0}^{i-1} \left(\frac{1}{2} - j \right) \right] \right. \\ &\quad \times \left. \left[\sum_{i=\lfloor \frac{n+k-l+1}{2} \rfloor}^{n+k-l} \hat{A}_{n+k-l-i}^i x^{2i-n-k+l} (-2)^i (1 - x^2)^{n-\frac{1}{2}-i} \prod_{j=0}^{i-1} \left(n - \frac{1}{2} - j \right) \right] \right\} \end{aligned} \quad (44)$$

with coefficients $\hat{A}_k^i$ given by (22).

A Fortran program of (44) is created. A few sample calculations illustrating the method are included in Table 2. The results are compared to Maple 11's output with 18 correct digits in the evalf command.

3.4. Application to Hermite functions

Normalized Hermite functions are defined as [28]:

$$\psi_n(x) = \frac{e^{-x^2/2}}{\sqrt{n!2^n\sqrt{\pi}}} H_n(x), \quad (45)$$

Table 2Numerical evaluation of $\frac{d^k}{dx^k} T_n(x)$, with $(n, x) = (8, 0.25)$.

k	Formula (44)	Values ^{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 3Numerical evaluation of $\frac{d^k}{dx^k} \psi_n(x)$, with $(n, x) = (5, 2)$.

k	Formula (49)	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)

where the Hermite polynomials $H_n(x)$ are defined as [28]:

$$H_n(x) = (-1)^n e^{x^2} \frac{d^n}{dx^n} e^{-x^2}. \quad (46)$$

Hermite polynomials satisfy the properties [28]:

$$\begin{cases} H_{n+1}(x) = 2xH_n(x) - 2nH_{n-1}(x) \\ \frac{d^i}{dx^i} H_n(x) = 2^i H_{n-i}(x) \prod_{j=0}^{i-1} (n-j), \end{cases} \quad (47)$$

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

$$\frac{d^k}{dx^k} e^{-x^2/2} = e^{-x^2/2} \sum_{i=\lfloor \frac{k+1}{2} \rfloor}^k (-1)^i \hat{A}_k^i x^{2i-k}, \quad (48)$$

with coefficients $\hat{A}_k^i$ given by (22).

Therefore, with the help of the Leibniz Formula (Formula 2.1) and Eq. (48), higher order derivatives of $\psi_n(x)$ are given by:

$$\frac{d^k}{dx^k} \psi_n(x) = \frac{e^{-x^2/2}}{\sqrt{n!2^n\sqrt{\pi}}} \sum_{l=0}^k \binom{k}{l} \left[\sum_{i=\lfloor \frac{l+1}{2} \rfloor}^l (-1)^i \hat{A}_l^i x^{2i-l} 2^{k-l} H_{n-k+l}(x) \prod_{j=0}^{k-l-1} (n-j) \right]. \quad (49)$$

A Fortran program of (49) is created. A few sample calculations illustrating the method are included in Table 3. The results are compared to Maple 11's output with 18 correct digits in the evalf command.

3.5. Application to 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 coordinates:

$$x^2 f''(x) + x f'(x) + (v^2 x^2 - n^2) f(x) = 0 \quad \text{in cylindrical coordinates,} \quad (50)$$

$$x^2 f''(x) + 2x f'(x) + (v^2 x^2 - n(n+1)) f(x) = 0 \quad \text{in spherical coordinates.} \quad (51)$$

In the literature [28], the normal convention adopted for representing Bessel functions arising in cylindrical and spherical coordinates, is given in the following Table:

Kind	Cylindrical	Spherical
First	$J_n(vx)$	$j_n(vx)$
Second	$Y_n(vx)$	$y_n(vx)$
Modified first	$I_n(vx)$	$i_n(vx)$
Modified second	$K_n(vx)$	$k_n(vx)$

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 (50) or (51), 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:

$$c_n(vx) = \sqrt{\frac{\pi}{2vx}} C_{n+1/2}(vx), \quad (52)$$

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 [28] to solve (50), Bessel functions of the first kind are expressed as:

$$J_n(vx) = \sum_{k=0}^{\infty} \frac{(-1)^k}{k! \Gamma(k+n+1)} \left(\frac{vx}{2}\right)^{2k+n}, \quad (53)$$

although there are many more numerically stable formulae that exist. One remarkably numerically stable formulation, as developed in [30], 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 $J_n(vx)$, $Y_n(vx)$, $K_n(vx)$, $j_n(vx)$, $y_n(vx)$ and $k_n(vx)$ is given by:

$$C'_n(vx) = \frac{n}{x} C_n(vx) - v C_{n+1}(vx). \quad (54)$$

This equation can be generalized as:

$$C_{n+k}(vx) = (-1)^k \frac{x^{n+k}}{v^k} \left(\frac{d}{xdx}\right)^k (x^{-n} C_n(vx)). \quad (55)$$

We are now ready to apply Theorem 3.1 with $(\mu, v, m, n) = (0, 0, 1, n)$ to obtain:

$$\frac{d^k}{dx^k} C_n(vx) = \sum_{i=0}^k (-1)^i \frac{v^i C_{n+i}(vx)}{x^{k-i}} A_k^i, \quad (56)$$

with coefficients A_k^i given by (7).

The Bessel derivative recurrence relation valid for $I_n(vx)$ and $i_n(vx)$:

$$\tilde{C}'_n(vx) = \frac{n}{x} \tilde{C}_n(vx) + v \tilde{C}_{n+1}(vx), \quad (57)$$

gives a similar result:

$$\tilde{C}_{n+k}(vx) = \frac{x^{n+k}}{v^k} \left(\frac{d}{xdx}\right)^k (x^{-n} \tilde{C}_n(vx)), \quad (58)$$

which, after application of Theorem 3.1 with $(\mu, v, m, n) = (0, 0, 1, n)$, yields:

$$\frac{d^k}{dx^k} \tilde{C}_n(vx) = \sum_{i=0}^k \frac{v^i \tilde{C}_{n+i}(vx)}{x^{k-i}} A_k^i, \quad (59)$$

with the same coefficients A_k^i . A few sample calculations illustrating the method applied to $j_n(vx)$, $I_n(vx)$, $k_n(vx)$ and $Y_n(vx)$ are included in Tables 4–7. The computation of the Bessel functions is performed using the programs presented in [31]. The

Table 4Numerical evaluation of $\frac{d^k}{dx^k} j_n(vx)$, with $(n, v, x) = (1, 1, 1)$.

k	Formula (56) ^a	evalf[15] ^a	evalf[22] ^a	evalf[28] ^a	Values ^{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)

^a Relative Error of given formula with respect to Values^{evalf[64]}.**Table 5**Numerical evaluation of $\frac{d^k}{dx^k} I_n(vx)$, with $(n, v, x) = (1, 1, 1)$.

k	Formula (59) ^a	evalf[15] ^a	evalf[22] ^a	evalf[28] ^a	Values ^{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)

^a Relative error of given formula with respect to Values^{evalf[64]}.

results are compared to Maple 11's output with different values of correct digits in the evalf command. In Tables 4–7, 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 [32], 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 [33], there exist a few other formulae for higher order derivatives of Bessel functions. None of these is, however, as concise or as general as (56) and (59). In addition, these formulae often require evaluation of hypergeometric series, while our formulae do not.

4. Treatment of differential equations

Theorem 4.1. For a function $f(x)$ satisfying an m th order linear homogeneous differential equation of the form:

$$f(x) = \sum_{k=1}^m p_k(x) \frac{d^k}{dx^k} f(x), \quad (60)$$

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

$$f(x^{\mu+1}) = \sum_{i=1}^m \bar{p}_i(x) \frac{d^i}{dx^i} f(x^{\mu+1}), \quad (61)$$

where:

$$\bar{p}_i(x) = \sum_{k=i}^m \frac{p_k(x^{\mu+1})}{(\mu+1)^k} x^{i-k(\mu+1)} \sum_{j=0}^i \frac{(-1)^{i-j} (j - (k-1)(\mu+1))_{k,\mu+1}}{j!(i-j)!}. \quad (62)$$

Proof. By making the substitution $x \leftrightarrow x^{\mu+1}$ in the differential equation (60), we obtain:

$$\begin{aligned} f(x^{\mu+1}) &= \sum_{k=1}^m p_k(x^{\mu+1}) \frac{d^k}{d(x^{\mu+1})^k} f(x^{\mu+1}) \\ &= \sum_{k=1}^m \frac{p_k(x^{\mu+1})}{(\mu+1)^k} \left(\frac{d}{x^{\mu} dx} \right)^k f(x^{\mu+1}) \\ &= \sum_{k=1}^m \frac{p_k(x^{\mu+1})}{(\mu+1)^k} \sum_{i=1}^k A_k^i x^{i-k(\mu+1)} \frac{d^i}{dx^i} f(x^{\mu+1}), \end{aligned} \quad (63)$$

where we have employed Theorem 3.1 with $(\mu, v, m, n) = (\mu, 0, 0, 0)$ in the last step, and where it is important to note that $A_k^0 = 0$ for $k > 0$ for this specific case.

Table 6Numerical evaluation of $\frac{d^k}{dx^k} k_n(vx)$, with $(n, v, x) = (1, 1, 1)$.

k	Formula (56) ^a	evalf[15] ^a	evalf[22] ^a	evalf[28] ^a	Values ^{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)

^a Relative error of given formula with respect to Values^{evalf[64]}.**Table 7**Numerical evaluation of $\frac{d^k}{dx^k} Y_n(vx)$, with $(n, v, x) = (1, 1, 1)$.

k	Formula (56) ^a	evalf[15] ^a	evalf[22] ^a	evalf[28] ^a	Values ^{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)

^a Relative error of given formula with respect to Values^{evalf[64]}.

By reversing the order of summation, we have:

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

and we obtain (61) and (62) by replacing coefficients A_k^i by their analytical expression (8) and by defining $\bar{p}_i(x)$ as the summation over k . $\square$

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

As an example of application of Theorem 4.1, we solve the second order linear differential equation:

$$f(x) = \left(\frac{1}{9x^5} - \frac{1}{3x^2} \right) \frac{d}{dx} f(x) - \frac{1}{18x^4} \frac{d^2}{dx^2} f(x), \quad (64)$$

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:

$$\bar{p}_1(x) = \frac{1}{9(\mu+1)x^{6\mu+5}} - \frac{1}{3(\mu+1)x^{3\mu+2}} + \frac{\mu}{18(\mu+1)^2 x^{6\mu+5}} \quad (65)$$

$$\bar{p}_2(x) = \frac{-1}{18(\mu+1)^2 x^{6\mu+4}}, \quad (66)$$

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

$$f\left(x^{\frac{1}{3}}\right) = -\frac{d}{dx} f\left(x^{\frac{1}{3}}\right) - \frac{1}{2} \frac{d^2}{dx^2} f\left(x^{\frac{1}{3}}\right), \quad (67)$$

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:

$$f(x) = e^{-x^3} (a \sin(x^3) + b \cos(x^3)), \quad (68)$$

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 4.1, 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.

4.1. 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 [8–13]. As part of the envelope of the spherical Bessel integral functions, reduced Bessel functions $\hat{k}_{n-\frac{1}{2}}(x)$ are defined as [34]:

$$\hat{k}_{n-\frac{1}{2}}(x) = \sqrt{\frac{2}{\pi}} x^{n-\frac{1}{2}} K_{n-\frac{1}{2}}(x) = \sum_{j=1}^n \frac{(2n-j-1)!}{(j-1)!(n-j)!} \frac{x^{j-1} e^{-x}}{2^{n-1}}, \quad (69)$$

and satisfy the differential equation:

$$\hat{k}_{n-\frac{1}{2}}(x) = -\frac{2(n-1)}{x} \frac{d}{dx} \hat{k}_{n-\frac{1}{2}}(x) + \frac{d^2}{dx^2} \hat{k}_{n-\frac{1}{2}}(x). \quad (70)$$

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 $x \rightarrow \infty$:

$$\gamma(x) = \sum_{n=0}^{\infty} \binom{1/2}{n} \frac{\tau^n}{\kappa^{n-\frac{1}{2}} x^{2n-1}} = x\sqrt{\kappa} \left(1 + \frac{\tau}{2\kappa x^2} - \frac{\tau^2}{8\kappa^2 x^4} + \cdots \right), \quad (71)$$

the asymptotic behaviour of the coefficients in (70) 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 $x \rightarrow \infty$ (For $n = 1$, $\bar{p}_1(x) \sim 1$ and $\bar{p}_2(x) = 0$ as $x \rightarrow \infty$). This result follows naturally from the development of Theorem 4.1 and the subsequent remark, but would have been difficult to obtain by hand.

5. Numerical integration

Let us consider the following semi-infinite highly oscillatory integrals:

$$\mathcal{I} = \int_0^{+\infty} \frac{x^{n_x}}{(\alpha^2 + x^2)^{k_1} (\beta^2 + x^2)^{k_2}} j_{\lambda}(vx) dx \quad (72)$$

$$= \sum_{n=0}^{+\infty} \int_{j_{\lambda,v}^n}^{j_{\lambda,v}^{n+1}} \frac{x^{n_x}}{(\alpha^2 + x^2)^{k_1} (\beta^2 + x^2)^{k_2}} j_{\lambda}(vx) dx \quad (73)$$

where α, β and v are positive real numbers, n_x, k_1 and k_2 are positive integers, and $j_{\lambda,v}^0 = 0$ and $j_{\lambda,v}^n$ for $n = 1, 2, \dots$ are the successive positive zeros of $j_{\lambda}(vx)$.

The semi-infinite integrals $\mathcal{I}$, which are to be evaluated via a numerical quadrature of integral representations in terms of nonphysical integration variables, are involved in the expressions of overlap integrals when the Fourier transform method is used [35]. These overlap integrals appear in molecular structure calculations.

The main difficulty in the numerical treatment of $\mathcal{I}$ is due to the presence of the spherical Bessel functions $j_{\lambda}(vx)$ in the integrands. As it is well known, the numerical integration of oscillatory integrands is beset with difficulties, especially when the oscillatory part is a spherical Bessel function and not a simple trigonometric function.

The spherical Bessel function is given by:

$$j_{\lambda}(x) = (-1)^{\lambda} x^{\lambda} \left(\frac{d}{xdx} \right)^{\lambda} \left[\frac{\sin(x)}{x} \right]. \quad (74)$$

Applying the Slevinsky–Safouhi formula I to the RHS of (74), with $(\mu, \nu, m, n) = (1, 1, 0, 0)$, we obtain:

$$j_{\lambda}(x) = (-1)^{\lambda} x^{\lambda} \sum_{i=0}^{\lambda} A_{\lambda}^i x^{i-2\lambda-1} \frac{d^i}{dx^i} \sin(x), \quad (75)$$

where the coefficients A_{λ}^i are given by Eq. (7).

Eq. (75) is equivalent to the following existing equation [36]:

$$j_{\lambda}(x) = \sum_{n=0}^{\lfloor \frac{\lambda}{2} \rfloor} \frac{(-1)^n (\lambda + 2n)!}{(2n)! (\lambda - 2n)!} \left(\frac{\sin(x - \frac{\lambda}{2}\pi)}{x(2x)^{2n}} \right) + \sum_{n=0}^{\lfloor \frac{\lambda-1}{2} \rfloor} \frac{(-1)^n (\lambda + 2n + 1)!}{(2n + 1)! (\lambda - 2n - 1)!} \left(\frac{\cos(x - \frac{\lambda}{2}\pi)}{x(2x)^{2n+1}} \right), \quad (76)$$

but it is worth noting that there is an advantage of using (75), which is the existence of recurrence relations (7) satisfied by the coefficients A_{λ}^i .

Table 8Numerical evaluation of the semi-infinite integral $\mathcal{I}$ (72). $\alpha = .35$, $\beta = .15$ and $v = 70.0$.

n_x	k_1	k_2	λ	$\mathcal{I}$	Error ⁽⁷³⁾	Error ⁽⁷⁸⁾	Error ⁽⁷⁹⁾
3	1	2	2	.635034253697001(−2)	.10(−14)	.20(−14)	.11(−14)
4	2	1	3	.968973803563365(−4)	.19(−13)	.18(−13)	.27(−15)
5	2	2	5	.152161419813517(−2)	.96(−15)	.48(−15)	.35(−15)
6	2	2	5	.848875335450666(−4)	.18(−13)	.19(−13)	.53(−15)
7	3	2	7	.316786693710785(−3)	.18(−15)	.19(−15)	.51(−15)
8	3	3	8	.204307627372025(−2)	.77(−15)	.41(−15)	.49(−15)
9	3	3	8	.205402825063235(−3)	.79(−15)	.90(−15)	.33(−15)

Total Calculation time using the infinite series with spherical Bessel functions = 1.4.

Total Calculation time using the infinite series with sine and cosine functions

Inserting Eq. (75) in the semi-infinite integral (72), we obtain:

$$\mathcal{I} = \frac{(-1)^\lambda}{v^{\lambda+1}} \sum_{i=0}^{\lambda} A_{\lambda}^i v^i \int_0^{+\infty} \frac{x^{n_x+i-\lambda-1}}{(\alpha^2 + x^2)^{k_1} (\beta^2 + x^2)^{k_2}} \sin\left(vx + i\frac{\pi}{2}\right) dx \quad (77)$$

$$= \frac{(-1)^\lambda}{v^{\lambda+1}} \sum_{i=0}^{\lambda} A_{\lambda}^i v^i \sum_{n=0}^{+\infty} \int_{x_{n,i}}^{x_{n+1,i}} \frac{x^{n_x+i-\lambda-1}}{(\alpha^2 + x^2)^{k_1} (\beta^2 + x^2)^{k_2}} \sin\left(vx + i\frac{\pi}{2}\right) dx, \quad (78)$$

where $x_{n,i}$ for $i = 0, 1, 2, \dots, \lambda$ and $n = 0, 1, 2, \dots$ are the positive successive zeros of $\sin\left(vx + i\frac{\pi}{2}\right)$ and they are given by $x_{0,i} = 0$ and for $n > 0$:

$$\begin{cases} x_{n,i} = \left(l - \frac{1}{2}\right) \frac{\pi}{v} & \text{if } i \text{ is odd} \\ x_{n,i} = l \frac{\pi}{v} & \text{if } i \text{ is even.} \end{cases}$$

By using the Slevinsky–Safouhi formula I, we transformed $\mathcal{I}$ into a finite linear combination of integrals involving successive derivatives of the sine function. These new integrals are easier to evaluate rapidly to a high pre-determined accuracy, due to practical properties of sine and cosine functions (mainly the fact that the successive zeros are equidistant).

The use of the infinite series (78) in the evaluation $\mathcal{I}$ reduces the calculation time by a factor 1.4 over the infinite series (73). In the case of more complicated spherical Bessel integrals, the transformation leads to a remarkable reduction of the calculation time.

One can easily demonstrate that the semi-infinite integrals involved in the above finite summation (77), which will be referred to as $\mathcal{I}_i$ ($0 \leq i \leq \lambda$), are suitable to apply $\bar{D}$ [37]. The successive zeros of the integrands are either the zeros of sine or cosine functions, and since they are equidistant one can use Cramer's rule for the computation of the approximations $\bar{D}_n^{(2)}$ of $\mathcal{I}_i$:

$$\bar{D}_n^{(2)} = \frac{\sum_{l=0}^{n+1} \binom{n+1}{l} \left(\frac{x_{1,i}}{\pi} + l\right)^{n-1} \left(\int_0^{x_{l+1,i}} \tilde{f}_i(t) dt\right) \frac{(\alpha^2 + x_{l+1,i}^2)^{k_1} (\beta^2 + x_{l+1,i}^2)^{k_2}}{x_{l+1,i}^{n_x+i-\lambda+1}}}{\sum_{l=0}^{n+1} \binom{n+1}{l} \left(\frac{x_{1,i}}{\pi} + l\right)^{n-1} \frac{(\alpha^2 + x_{l+1,i}^2)^{k_1} (\beta^2 + x_{l+1,i}^2)^{k_2}}{x_{l+1,i}^{n_x+i-\lambda+1}}}, \quad (79)$$

where $\tilde{f}_i(x)$ is the integrand of $\mathcal{I}_i$ for $i = 0, 1, \dots, \lambda$.

Recurrence relations were developed [10] for equations of the form given by (79). These recurrence relations allow the control of the degree of accuracy by comparing two successive approximations $\bar{D}_k^{(2)}$ and $\bar{D}_{k+1}^{(2)}$ until the pre-determined accuracy is reached. In Table 8, we list values of $\mathcal{I}$ (72) obtained using the infinite series (73) and (78) as well as $\bar{D}$ given by (79).

6. Numerical discussion

The implications of Theorem 3.1 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 $\left. \frac{d^{14}}{dx^{14}} j_n(vx) \right|_{(n,v,x)=(1,1,1)}$ 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 (56) or (59) 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 1–7, Theorem 3.1 is accurate to 15 correct digits evaluated in double precision. This implementation in Fortran is remarkable because all of the examples of Theorem 3.1 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 4 and 5 highlight the efficacy of (56) and (59), Tables 6 and 7 show their limitations, especially concerning the evaluation of the derivatives of $k_n(vx)$ and $Y_n(vx)$. Formula (56) does not achieve complete machine precision for these functions because for $(v, x) = (1, 1)$, (56) 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 $j_n(vx)$ because each term is not significantly larger or smaller than the previous one. This also does not occur when computing the derivatives of $I_n(vx)$, as (59) is not an alternating series. Interestingly, Maple 11 seems to show no difficulty computing the derivatives of $k_n(vx)$ or $Y_n(vx)$, the modified Bessel functions.

In Tables 1–3, we list the values obtained using the formulae (39), (44) and (49) respectively. In these tables, values with 18 correct digits are obtained using Maple 11 evalf[18] and they are referred to as Values^{evalf[18]}. In Tables 4–7, we list the relative errors with respect to values obtained using Maple 11 evalf[64], which are referred to as Values^{evalf[64]}. In these tables, we list the relative errors obtained using our formulae, Maple's evalf[15], evalf[22] and evalf[28]. In Table 8, we list the values of the semi-infinite integrals $\mathcal{I}$ (72). These values are obtained using the infinite series with spherical Bessel functions (73), the infinite series with sine and cosine functions (78) and the $\bar{D}$ transformation given by (79) with the recurrence relation presented in [10].

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

7. Conclusion

We present new formulae, which we called the Slevinsky–Safouhi formulae, for the analytical development of higher order derivatives. The formulae are analytic and exact and they represent the k th derivative as a discrete sum of only $k + 1$ terms. The coefficients involved in the summation can be computed recursively and they are not subject to any computational instability. We explicitly show how Theorem 3.1 is applicable to Legendre functions, Chebyshev polynomials of the first kind, Hermite functions, and Bessel functions. In addition, we also show the most general cases of Theorem 3.1, notably, $\frac{d^k}{dx^k}(x^n f(x^{m+1}))$, $\frac{d^k}{dx^k}(x^n f(\ln(x)))$, and $\frac{d^k}{dx^k}(e^{nx} f(e^x))$. Theorem 4.1 proves to be a useful tool for solving and/or characterizing certain classes of differential equations.

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