

USING INTEGRAL TRANSFORMS TO ESTIMATE HIGHER ORDER DERIVATIVES

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1. INTRODUCTION

When doing error analysis for numerical quadrature, achieving good uniform bounds on higher order derivatives of the integrand is paramount. As undergraduates become increasingly adept with programmable calculators, numerical integration schemes such as Simpson's Rule and the Trapezoidal Rule take on a new relevance. Although it may be a rare calculus class that dwells overmuch on error bounds for such schemes, this may be due as much to the perceived paucity of interesting examples for which decent error bounds are readily achievable as to the general weakness in algebraic skills necessary for the requisite understanding of inequalities. The purpose of this article, therefore, is to offer some interesting, non-trivial examples for which the error analysis, if not elegant, is at least simple enough to carry out in the classroom.

2. THE SINE, COSINE AND EXPONENTIAL INTEGRALS

The sine integral ([1, pp. 231–232] or [12, pp. 503–504]) is given by

$$\text{Si}(x) = \int_0^x \frac{\sin t}{t} dt. \quad (2.1)$$

The integrand of (2.1) is a scaled version of the sinc function, as it is referred to by those who work on problems involved with signal processing and reconstruction. Thus, $\text{sinc}(t) = \sin(\pi t)/(\pi t)$ for $t \neq 0$, and it is convenient to define $\sin 0/0 = 1$, thereby removing the removable discontinuity. For Simpson's rule, we require a good uniform upper bound on the absolute value of the fourth derivative of the integrand ([1, p. 886] or [5, pp. 57–58]). Repeated application of the product rule for differentiation gives

$$\left(\frac{d}{dt}\right)^4 \frac{\sin t}{t} = \frac{\sin t}{t} + \frac{4 \cos t}{t^2} - \frac{12 \sin t}{t^3} - \frac{24 \cos t}{t^4} + \frac{24 \sin t}{t^5},$$

which in this form is difficult to estimate, not only because of the complicated nature of the formula, but also because of the apparent difficulties when t is near zero. However,

$$\frac{\sin t}{t} = \int_0^1 \cos(st) ds, \quad (2.2)$$

Date: Submitted June 1, 1999. Revised August 17, 1999.

1991 Mathematics Subject Classification. Primary: 44A20; Secondary: 65D30, 65R10.

Key words and phrases. Integral Transforms, Simpson's Rule, Estimating Derivatives, Differentiating under the Integral Sign.

and hence by Leibniz's rule for differentiating under the integral sign,

$$\left(\frac{d}{dt}\right)^4 \frac{\sin t}{t} = \int_0^1 s^4 \cos(st) ds. \quad (2.3)$$

Since $|\cos(st)| \leq 1$ for all real s and t , it follows that

$$\left|\left(\frac{d}{dt}\right)^4 \frac{\sin t}{t}\right| \leq \int_0^1 s^4 ds = \frac{1}{5}. \quad (2.4)$$

The inequality is sharp, as can be seen by substituting $t = 0$ in (2.3). In a similar manner, one can show that for all nonnegative integers k ,

$$\left|\left(\frac{d}{dt}\right)^k \frac{\sin t}{t}\right| \leq \int_0^1 s^k ds = \frac{1}{k+1}, \quad (2.5)$$

with equality at $t = 0$ when k is even. Instead of starting with (2.2), an analysis based on the equivalent representation

$$\frac{\sin t}{t} = \frac{1}{2} \int_{-1}^1 e^{ist} ds \quad (2.6)$$

can likewise be given, although in freshman/sophomore calculus classes it is less likely that students will be comfortable with the complex exponential.

For the cosine integrals ([1, pp. 231–232] or [12, pp. 503–504])

$$\text{Cin}(x) = \int_0^x \frac{1 - \cos t}{t} dt, \quad \text{Ci}(x) = \gamma + \log x + \int_0^x \frac{\cos t - 1}{t} dt, \quad (2.7)$$

we define the integrand to be zero when $t = 0$ so that for all real t ,

$$\frac{1 - \cos t}{t} = \int_0^1 \sin(st) ds, \quad (2.8)$$

and hence

$$\left(\frac{d}{dt}\right)^4 \frac{1 - \cos t}{t} = \int_0^1 s^4 \sin(st) ds.$$

Since $|\sin(st)| \leq 1$ for all real s and t , it follows that

$$\left|\left(\frac{d}{dt}\right)^4 \frac{1 - \cos t}{t}\right| \leq \int_0^1 s^4 ds = \frac{1}{5}, \quad (2.9)$$

and in general, for all nonnegative integers k ,

$$\left|\left(\frac{d}{dt}\right)^k \frac{1 - \cos t}{t}\right| \leq \int_0^1 s^k ds = \frac{1}{k+1}, \quad (2.10)$$

with equality at $t = 0$ when k is odd.

The hyperbolic sine and cosine integrals ([1, p. 231] or [7, p. 936])

$$\begin{aligned} \text{Shi}(x) &= \int_0^x \frac{\sinh t}{t} dt, \\ \text{Cinh}(x) &= \int_0^x \frac{1 - \cosh t}{t} dt, \\ \text{Chi}(x) &= \gamma + \log x + \int_0^x \frac{\cosh t - 1}{t} dt, \quad x > 0 \end{aligned}$$

can be treated in much the same way. For example, for Shi one replaces \sin by \sinh and \cos by \cosh in (2.1)–(2.3). The bound in (2.5) is modified by the presence of an extra factor of $\cosh t$ or $|\sinh t|$ according to whether k is even or odd. In either case, equality obtains when $t = 0$.

The exponential integral ([1, pp. 228–231] or [12, pp. 504–505])

$$E_1(x) = \int_1^\infty \frac{e^{-xt}}{t} dt, \quad x > 0 \quad (2.11)$$

is another natural choice to study using this technique. In this case, it is easier to deal with the complementary expression

$$\text{Ein}(x) = \int_0^x \frac{1 - e^{-t}}{t} dt, \quad (2.12)$$

since the latter defines an entire function. In view of the relationship ([1, p. 228] or [9, p. 40])

$$\text{Ein}(x) = \log x + \gamma + E_1(x), \quad x > 0,$$

there is no essential difference between the two. If we define the integrand of (2.12) to be zero when $t = 0$, then

$$\frac{1 - e^{-t}}{t} = \int_0^1 e^{-st} ds, \quad \left(\frac{d}{dt}\right)^k \frac{1 - e^{-t}}{t} = \int_0^1 (-s)^k e^{-st} ds, \quad (2.13)$$

and so for $t \geq 0$ and k a nonnegative integer,

$$\left| \left(\frac{d}{dt}\right)^k \frac{1 - e^{-t}}{t} \right| = \int_0^1 s^k e^{-st} ds \leq \int_0^1 s^k ds = \frac{1}{k+1}, \quad (2.14)$$

with equality again when $t = 0$.

3. HOW GOOD ARE THESE ESTIMATES IN PRACTICE?

The estimates (2.4) and (2.14) of the previous section are best possible in the sense that equality holds in each when $t = 0$. On the other hand, the corresponding derivatives (2.3) and (2.13) each tend to zero as t grows without bound, so it is clear that a uniform numerical bound for the entire range of t values is less than ideal. Nevertheless, it is instructive to see just how well our estimates hold up in practice. We confine ourselves here to a single example, the cosine integral, in which we test the inequality (2.9) used to give an error estimate for Simpson's Rule against the error arising from an actual computation.

Let $f : \mathbf{R} \rightarrow \mathbf{R}$ be given by $f(0) = 0$ and $f(t) = (1 - \cos t)/t$ for $t \neq 0$. Then the cosine integral (2.7) is given by

$$\text{Cin}(x) = \int_0^x f(t) dt. \quad (3.1)$$

For even positive integers n and real $x > 0$, define

$$S_n(x) := \frac{x}{3n} \left\{ f(0) + 4 \sum_{j=1}^{n/2} f\left(\frac{(2j-1)x}{n}\right) + 2 \sum_{j=1}^{n/2-1} f\left(\frac{2jx}{n}\right) + f(x) \right\},$$

the approximation to the integral (3.1) obtained by applying Simpson's Rule with n subdivisions of the interval $[0, x]$. The error is given by [5, p. 58]

$$E_n(x) := S_n(x) - \text{Cin}(x) = \frac{x^5 f^{(4)}(\xi)}{180n^4},$$

where $\xi = \xi(x) \in [0, x]$. In view of (2.9), we have the inequality

$$|E_n(x)| \leq B_n(x), \quad \text{where} \quad B_n(x) := \frac{x^5}{900n^4}. \quad (3.2)$$

To compare the estimate B_n with the actual error E_n , we let

$$R_n(x) := \frac{B_n(x)}{E_n(x)} = \frac{B_n(x)}{S_n(x) - \text{Cin}(x)}$$

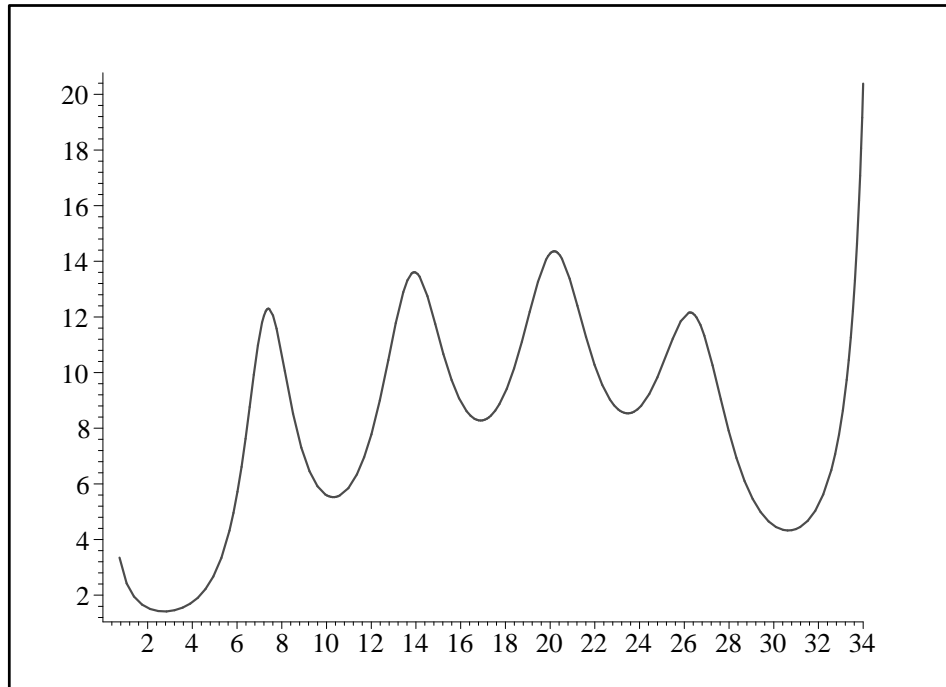
be the ratio of the two quantities. Then R_n is defined except for those points at which the actual error vanishes, and elsewhere $|R_n| \geq 1$.

Using Maple's built-in cosine integral, it is possible, in principle, to compute E_n (and hence R_n) to any desired precision. Table 1 gives an indication of the range of values of $R_n(x)$ for $0 \leq x \leq 10$. Tabular values were computed using Maple V Release 5 with a conservative working precision of twenty decimal places. Entries were then rounded to two decimal places to make comparison easier. Thus, for example, the error bound given by (3.2) arising from the estimate (2.9) exceeds the actual error by a factor of almost 3 when $x = 5$ and Simpson's Rule is used with $n = 10, 100$, or 1000 subdivisions. When $x = 7$, the corresponding overestimate is by a factor of less than 12.

$x \setminus n$	10	100	1000
1.0	2.55	2.56	2.56
2.0	1.54	1.55	1.55
3.0	1.43	1.44	1.44
4.0	1.75	1.77	1.77
5.0	2.77	2.82	2.82
6.0	5.63	5.75	5.75
7.0	11.31	11.58	11.58
8.0	10.66	11.18	11.18
9.0	6.97	7.51	7.51
10.0	5.59	6.14	6.15

TABLE 1. Values of $R_n(x)$

Figure 1 is a graph of $R_{10}(x)$ for $0 \leq x \leq 34$, and makes it clear that there is nothing special about our choice of integer values for x in Table 1. We see that for $0 \leq x \leq 20$, $1 \leq R_{10}(x) \leq 15$, i.e. the bound (3.2) is never farther than a factor of 15 from the truth on the interval $[0, 20]$. Beyond $x = 30$, we see what appears to be the formation of a spike in the graph. This is best explained by the computed values $E_{10}(34.858) = 0.00016504\dots$ and $E_{10}(34.859) = -0.000095463\dots$. Since the actual error E_{10} is clearly a continuous function, the intermediate value theorem implies that E_{10} vanishes at some point in the interval $[34.858, 34.859]$. On the other hand, the estimated error B_{10} is clearly an increasing function, so it follows that there exist exceptional tiny intervals on which the estimated error

FIGURE 1. Graph of $R_{10}(x)$

overestimates the actual error by arbitrarily large factors. However, this kind of phenomenon is in general to be expected for Simpson's Rule no matter what sort of error estimate is used (apart from one based on the actual error function itself!)

4. UNDERSTANDING THE EXAMPLES

Although the reasoning of Section 2 may be easy to follow, the student might legitimately wonder how one arrives at useful integral representations such as (2.2), (2.6), (2.8), or (2.13) in the first place. We begin by observing that the examples of Section 2 deal with integrands of the form $(f(t) - f(0))/t$. More generally, if $f : [a, b] \rightarrow \mathbf{R}$ has $n+1$ continuous derivatives, repeated integration by parts applied to the equation

$$f(t) = f(a) + \int_a^t f'(u) du$$

yields Taylor's formula with the integral form of the remainder:

$$f(t) = \sum_{j=0}^n \frac{(t-a)^j}{j!} f^{(j)}(a) + \int_a^t \frac{(t-u)^n}{n!} f^{(n+1)}(u) du, \quad a < t < b. \quad (4.1)$$

If we make the change of variable $u = (t-a)s + a$ and rearrange (4.1), we obtain

$$\frac{f(t) - \sum_{j=0}^n \frac{(t-a)^j f^{(j)}(a)}{j!}}{(t-a)^{n+1}} = \int_0^1 \frac{(1-s)^n}{n!} f^{(n+1)}((t-a)s + a) ds, \quad (4.2)$$

and hence if f is sufficiently differentiable, Leibniz's rule for differentiating under the integral sign yields

$$\begin{aligned} \left(\frac{d}{dt}\right)^k \frac{f(t) - \sum_{j=0}^n (t-a)^j f^{(j)}(a)/j!}{(t-a)^{n+1}} \\ = \frac{1}{n!} \int_0^1 s^k (1-s)^n f^{(n+k+1)}((t-a)s+a) ds. \end{aligned} \quad (4.3)$$

If a uniform upper bound on the absolute value of the derivative of f of order $n+k+1$ is known, say

$$\sup_{a \leq t \leq b} |f^{(n+k+1)}(t)| \leq M, \quad (4.4)$$

then we have the upper bound

$$\frac{M}{n!} \int_0^1 s^k (1-s)^n ds = \frac{k! M}{(n+k+1)!} \quad (4.5)$$

for the absolute value of the left hand side of (4.3), i.e.,

$$\left| \left(\frac{d}{dt}\right)^k \frac{f(t) - \sum_{j=0}^n (t-a)^j f^{(j)}(a)/j!}{(t-a)^{n+1}} \right| \leq \frac{k! M}{(n+k+1)!}. \quad (4.6)$$

It is readily apparent that (2.5), (2.10), and (2.14) are special cases of (4.6) in which $a = n = 0$ and $f(t) = \sin t$, $f(t) = -\cos t$, and $f(t) = -\exp(-t)$, respectively.

For an example with $n > 0$, consider

$$\int_0^x \frac{1 - \cos t}{t^2} dt,$$

which arises in the study of incomplete versions of the Frullani integral ([7, p. 470] or [12, p. 398])

$$\begin{aligned} \int_0^\infty \frac{\cos \alpha t - \cos \beta t}{t^2} dt &= \int_0^\infty \left(\frac{1 - \cos \beta t}{t^2} - \frac{1 - \cos \alpha t}{t^2} \right) dt \\ &= (|\beta| - |\alpha|) \frac{\pi}{2}, \quad \alpha, \beta \in \mathbf{R}. \end{aligned}$$

Repeated application of the product rule for differentiation gives

$$\left(\frac{d}{dt}\right)^4 \frac{1 - \cos t}{t^2} = \frac{120(1 - \cos t)}{t^6} - \frac{96 \sin t}{t^5} + \frac{36 \cos t}{t^4} + \frac{8 \sin t}{t^3} - \frac{\cos t}{t^2},$$

which again, is troublesome to estimate as it stands. On the other hand, (4.3) with $f(t) = \cos t$, $n = 1$, $a = 0$, and $k = 4$ gives

$$\left(\frac{d}{dt}\right)^4 \frac{1 - \cos t}{t^2} = \int_0^1 s^4 (1-s) \cos(st) ds,$$

whence

$$\left| \left(\frac{d}{dt}\right)^4 \frac{1 - \cos t}{t^2} \right| \leq \int_0^1 s^4 (1-s) ds = \frac{1}{30},$$

with equality at $t = 0$. More generally, (4.4) with $M = 1$ is satisfied when $f(t) = \cos t$, and so (4.5) and (4.6) give

$$\left| \left(\frac{d}{dt} \right)^k \frac{1 - \cos t}{t^2} \right| \leq \int_0^1 s^k (1 - s) ds = \frac{1}{(k+1)(k+2)},$$

with equality at $t = 0$ when k is even.

5. SOME MORE SOPHISTICATED EXAMPLES

The inverse tangent integral

$$\text{Ti}_2(x) = \int_0^x \frac{\tan^{-1}(t)}{t} dt,$$

would appear to be another example amenable to our technique. Lewin [8, chapter 2] devotes a whole chapter to the study of its properties. The inverse tangent integral evidently also attracted the interest of Ramanujan [10], who among other things used it to develop a rapidly convergent series of hyperbolic functions for Catalan's constant, $\text{Ti}_2(1)$ ([1, p. 807], [4]). Formula (4.2) with $a = n = 0$ and $f(t) = \tan^{-1}(t)$ yields

$$\frac{\tan^{-1}(t)}{t} = \int_0^1 \frac{ds}{1 + s^2 t^2}. \quad (5.1)$$

After differentiating under the integral and simplifying the resulting expression, one arrives at

$$\left(\frac{d}{dt} \right)^4 \frac{\tan^{-1}(t)}{t} = \int_0^1 \frac{24s^4(5s^4 t^4 - 10s^2 t^2 + 1)}{(1 + s^2 t^2)^5} ds. \quad (5.2)$$

It is difficult to obtain a good uniform estimate on the size of the integrand in (5.2), so we return to (5.1). After making the change of variable $s = 1/u$ and employing the formula

$$\int_0^\infty e^{-uv} \cos(vt) dv = \frac{u}{u^2 + t^2}, \quad u > 0,$$

an application of Fubini's theorem [6, p. 67] gives

$$\begin{aligned} \frac{\tan^{-1}(t)}{t} &= \int_1^\infty \frac{1}{u} \cdot \frac{u du}{u^2 + t^2} \\ &= \int_1^\infty \frac{1}{u} \int_0^\infty e^{-uv} \cos(vt) dv du \\ &= \int_0^\infty \int_1^\infty \frac{e^{-uv}}{u} du \cos(vt) dv \\ &= \int_0^\infty E_1(v) \cos(vt) dv, \end{aligned}$$

where E_1 is the exponential integral (2.11). Thus,

$$\left(\frac{d}{dt} \right)^4 \frac{\tan^{-1}(t)}{t} = \int_0^\infty v^4 E_1(v) \cos(vt) dv,$$

and hence by Tonelli's theorem [6, p. 67],

$$\begin{aligned}
\left| \left(\frac{d}{dt} \right)^4 \frac{\tan^{-1}(t)}{t} \right| &\leq \int_0^\infty v^4 E_1(v) dv \\
&= \int_0^\infty v^4 \int_1^\infty \frac{e^{-uv}}{u} du dv \\
&= \int_1^\infty \frac{1}{u} \int_0^\infty v^4 e^{-uv} dv du \\
&= 4! \int_1^\infty \frac{du}{u^6} \\
&= \frac{24}{5}.
\end{aligned}$$

In the same manner, it can be shown more generally that for all nonnegative integers k ,

$$\left| \left(\frac{d}{dt} \right)^k \frac{\tan^{-1}(t)}{t} \right| \leq \int_0^\infty v^k E_1(v) dv = \frac{k!}{k+1},$$

with equality at $t = 0$ when k is even.

The previous example gives an idea of what is possible when one steps outside the framework of Section 4. As another example, suppose one wanted to estimate the even derivatives of the tangent function. From [7, p. 388],

$$\tan t = 2 \int_0^\infty \frac{\sinh 2st}{\sinh \pi s} ds, \quad -\pi/2 < t < \pi/2.$$

It follows that for all nonnegative integers k , we have

$$\left(\frac{d}{dt} \right)^{2k} \tan t = 2 \int_0^\infty (2s)^{2k} \frac{\sinh 2st}{\sinh \pi s} ds, \quad -\pi/2 < t < \pi/2. \quad (5.3)$$

As s gets large, we expect

$$\frac{\sinh 2st}{\sinh \pi s} = \frac{e^{2st} - e^{-2st}}{e^{\pi s} - e^{-\pi s}}$$

to behave like $e^{(2t-\pi)s}$ for $0 < 2t < \pi$. In fact, it is easy to prove that the inequality

$$\frac{\sinh 2s|t|}{\sinh \pi s} \leq e^{(2|t|-\pi)s}$$

holds for $-\pi < 2t < \pi$ and $s > 0$. Therefore, by (5.3), we have

$$\left| \left(\frac{d}{dt} \right)^{2k} \tan t \right| \leq 2 \int_0^\infty (2s)^{2k} e^{(2|t|-\pi)s} ds = \frac{(2k)!}{(\pi/2 - |t|)^{2k+1}} \quad (5.4)$$

for all nonnegative integers k . The estimate (5.4) is remarkably good even when $|t|$ is small, with asymptotic equality in the limit as $|t| \rightarrow \pi/2^-$.

The previous two examples succeeded because we were able to represent the desired function as a Fourier (respectively, Laplace) transform of a well-behaved function. As a final example, consider the integral

$$\int_a^b t^{-2\kappa} e^{-ut} e^{\kappa \operatorname{Ein}(t)} dt, \quad (5.5)$$

in which $0 < a < b$, $\kappa > 1$, and $u > 0$ are real parameters, and Ein is the complementary exponential integral (2.12). The integral (5.5) arises in the solution of certain advanced argument difference-differential equations relating to sieves ([2], [3]), and as such, it is desirable to be able to compute it accurately for various values of the parameters. To study the integrand of (5.5), we let $c > 0$ and define

$$\lambda_\kappa(v) := \frac{1}{2\pi i} \int_{c-i\infty}^{c+i\infty} e^{vz} z^{-2\kappa} e^{\kappa \text{Ein}(z)} dz. \quad (5.6)$$

By Cauchy's theorem, the line integral (5.6) is independent of c , and vanishes for $v \leq 0$. It is not hard to show that λ_κ is continuous and satisfies the delay differential equation

$$(v^{1-\kappa} \lambda_\kappa(v))' = \kappa v^{-\kappa} \lambda_\kappa(v-1), \quad v > 0, \quad (5.7)$$

with boundary condition

$$\lambda_\kappa(v) = \frac{e^{\kappa v}}{\Gamma(\kappa)} v^{\kappa-1}, \quad 0 \leq v \leq 1. \quad (5.8)$$

Let $f(t)$ denote the integrand of (5.5). By Laplace inversion,

$$\int_0^\infty e^{-vt} \lambda_\kappa(v) dv = t^{-2\kappa} e^{\kappa \text{Ein}(t)}, \quad t > 0,$$

and differentiating under the integral sign to obtain

$$\begin{aligned} f^{(4)}(t) &= \left(\frac{d}{dt}\right)^4 t^{-2\kappa} e^{-ut} e^{\kappa \text{Ein}(t)} = \int_0^\infty (u+v)^4 e^{-(u+v)t} \lambda_\kappa(v) dv, \\ f^{(5)}(t) &= \left(\frac{d}{dt}\right)^5 t^{-2\kappa} e^{-ut} e^{\kappa \text{Ein}(t)} = - \int_0^\infty (u+v)^5 e^{-(u+v)t} \lambda_\kappa(v) dv, \end{aligned}$$

can be justified. But, the delay differential equation (5.7) and boundary condition (5.8) together show that λ_κ is nonnegative, and hence $f^{(4)}$ is nonnegative and nonincreasing. It follows that

$$\sup_{a \leq t \leq b} |f^{(4)}(t)| = f^{(4)}(a),$$

a considerable simplification.

6. CONCLUSION

Of course, there are other methods for bounding the derivatives of a suitable function, the most familiar of which is undoubtedly Cauchy's inequality (see eg. [11, p. 91]) from the theory of complex variables. One can also consider alternative approaches to error analysis which do not involve estimating higher order derivatives. Chapter 4 of Davis and Rabinowitz [5] is devoted to error analysis for various approximate integration schemes. In addition to a section on error estimates via analytic function theory, alluded to previously, there is a lovely section (see pp. 317–332) describing applications of functional analysis to numerical integration and error estimation.

In this paper, however, we have deliberately focused on the use of integral transforms arising primarily in the context of real variable theory. The technique can be summarized as follows: find a suitable integral representation for the function whose derivatives are to be estimated, differentiate under the integral sign, and estimate the resulting integral. The technique is hardly new, but is seldom used to

its fullest advantage. It is hoped that some of the examples provided herein could be used to enrich the discussion of numerical integration in a typical calculus or numerical analysis course.

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