Numerical Integration of Periodic Functions: A Few Examples

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1. A TEXTBOOK PROBLEM. In one of the more popular calculus textbooks the following problem appears [**13**, p. 466]:

This exercise deals with approximations to the integral

$$I(f) = \int_0^{2\pi} f(x)\,dx, \quad \textit{where} \quad f(x) = e^{\cos x}. \tag{1}$$

(*a*) *Use a graph to get a good upper bound for* $|f''(x)|$.

(*b*) *Use* M_{10} *to approximate* I.

(*c*) *Use part (a) to estimate the error in part (b).*

(*d*) *Use the built-in numerical integration capability of your CAS*[1] *to approximate* I.

(*e*) *How does the actual error compare with the error estimate in part (c)?*

The notation M_{10} in part (b) refers to the 10-panel midpoint rule for numerical integration. This is nothing but a Riemann sum in which the midpoint of each subinterval determines the height of the rectangle. That is, we partition the interval $[0, 2\pi]$ into N subintervals with uniform width $h = 2\pi/N$ by defining[2]

$$x_j = jh, \qquad j = 0, \ldots, N.$$

The midpoint rule $M_N(f)$ and its standard error estimate (to be used in part (c)) are then given as in Stewart [**13**, pp. 458–460] by

$$M_N(f) = h \sum_{j=0}^{N-1} f\left(x_j + \tfrac{1}{2}h\right), \qquad |I(f) - M_N(f)| \le \frac{\pi^3}{3}\frac{K}{N^2}. \tag{2}$$

The assumption is that $f(x)$ is at least twice continuously differentiable on $[0, 2\pi]$ and K is any bound on the magnitude of the second derivative, i.e.,

$$|f''(x)| \le K, \qquad 0 \le x \le 2\pi.$$

We also state the trapezoidal rule $T_N(f)$, with its error estimate[3]

$$T_N(f) = h\left(\tfrac{1}{2}f(0) + \sum_{j=1}^{N-1} f(x_j) + \tfrac{1}{2}f(2\pi)\right), \qquad |I(f) - T_N(f)| \le \frac{2\pi^3}{3}\frac{K}{N^2}. \tag{3}$$

The constant K has the same meaning as above.

[1] CAS = Computer Algebra System.

[2] The interval $[0, 2\pi]$ is for convenience only. Everything we say can easily be extended to an arbitrary interval $[a, b]$.

[3] One notices that the error bound for the midpoint rule is one half that of the trapezoidal rule; compare (2) with (3). For a pretty geometrical explanation of why one can expect the midpoint rule to be better by about a factor of two, the reader is referred to Stewart [**13**, p. 460].

Starting with part (a) of the textbook problem, we dutifully turn to our CASs, compute the second derivative (only the brave do this by hand), plot it on $[0, 2\pi]$, and observe that the maximum magnitude is reached at both $x = 0$ and $x = 2\pi$. We conclude that, if $f(x) = e^{\cos x}$, then

$$|f''(x)| \leq e \ (= 2.718\ldots),$$

which we record for use in part (c).

As for parts (b) and (d), we compute $I(f)$ and $M_{10}(f)$ as

$$I(f) \approx 7.954926521, \qquad M_{10}(f) \approx 7.954926518,$$

rounded to ten significant digits. (In Section 6 we compute $I(f)$ explicitly in terms of a special function.) The error is

$$I(f) - M_{10}(f) \approx 3 \times 10^{-9}, \tag{4}$$

which is spectacularly small considering the relatively small value of N.

The excitement turns to disappointment when we continue to parts (c) and (e). To work part (c) we use the error bound (2). We have established that the best bound for the second derivative is $K = e$, and with $N = 10$ we get

$$|I(f) - M_{10}(f)| \leq \frac{\pi^3}{3} \frac{e}{10^2} \approx 0.28. \tag{5}$$

True but useless, this bound overestimates the actual error (4) by a factor of about 10^8. It's like saying the distance between New York and London is less than 10^{11} miles (about a million times the circumference of the earth!).

At this point many teaching assistants and even a few professors find themselves at a loss for words to explain this spectacular failure of the error bound (2). The exceptions are the numerical analysts, who would be quick to point out that the midpoint rule (as well as the trapezoidal rule) is more accurate than usual when applied to integrate smooth periodic functions over one period. For such functions the convergence is so quick that the standard error estimate becomes irrelevant. This is illustrated in the following table.

N	$I(f) - M_N(f)$	Error bound (2)
4	3.4×10^{-2}	1.8×10^{0}
8	1.3×10^{-6}	4.4×10^{-1}
12	6.5×10^{-12}	2.0×10^{-1}

One of the things we intend to show here is that the actual error decays like[4]

$$I(f) - M_N(f) \sim 2\left(\frac{2\pi}{N}\right)^{1/2} \left(\frac{e}{2N}\right)^{N}, \tag{6}$$

which yields the estimates 3.3×10^{-2}, 1.2×10^{-6}, 6.4×10^{-12} when $N = 4, 8, 12$, respectively. These numbers compare favorably with the values listed in the middle column of the table, despite the fact that N is not particularly large.

[4]We use the notation $a_N \sim b_N$ to denote that $\lim_{N\to\infty} a_N/b_N = 1$.

2. PRELIMINARIES.

2. PRELIMINARIES. A general analysis of the speed of convergence of the midpoint and trapezoidal rules for smooth periodic functions requires a good dose of advanced calculus. In the literature one finds three approaches: (a) Fourier series [**7**, p. 155], (b) residue calculus [**9**, p. 211], and (c) the Euler-Maclaurin summation formula [**2**, p. 285].

All three of these approaches require background that the typical first-year calculus student lacks. For that matter, it cannot be taken for granted that a numerical analysis student at the junior or senior level will know much about these topics either. This leaves the instructor with only one recourse to explain the observed discrepancy between the actual error and the theoretical error bound: hand-waving.

The author's own effort goes something like this: "Interpret the integral as the area under the graph of $f(x)$, and consider the trapezoidal rule. In those regions where the graph is concave up (respectively, down) the trapezoids overestimate (respectively, underestimate) the true area. When the function is periodic and one integrates over one full period, there are about as many sections of the graph that are concave up as concave down, so the errors cancel. This leaves one with a much better approximation than would have been the case had the function been monotonic."

This explanation satisfies most students, and they go on their way to more interesting things. Thankfully, however, there are some students who would like to know more, and this note was written for them.

We shall present a series of examples, almost all of which have the property that the error in the trapezoidal and midpoint rules can be computed explicitly. These examples were selected to illustrate a variety of convergence behaviors, most of them quicker than the typical $1/N^2$ given by (2) and (3). We shall see algebraic convergence like $1/N^4$, geometric convergence like r^N (with $0 < r < 1$), as well as the superfast convergence described by (6). A complete list of examples, arranged in increasing order of speed of convergence, is given in Table 1. (All integrals are defined on $[0, 2\pi]$, and N is the number of subintervals in the integration rule.)

TABLE 1. Examples

Example	Essential convergence rate	Section
$f_2(x) = \sin(x/2)$	$1/N^2$	4
$f_7(x) = e^{-x^2}$	$1/N^2$	8
$f_3(x) = \sin^3(x/2)$	$1/N^4$	4
$f_6(x) = e^{(\cos x - 1)/(\cos x + 1)}$	$e^{-(3/2)N^{2/3}}$	7
$f_4(x) = 1/(a - \cos x)$, $a > 1$	r^N $(0 < r < 1)$	5
$f_5(x) = e^{a \cos x}$	$1/N^N$	6
$f_1(x) = \cos kx$, k an integer	exact $(N > k)$	3

Our principal aim was to write this paper in such a way that it may serve as supplementary reading for the first courses in integral calculus or numerical analysis. For this reason we shall present the examples in increasing order of mathematical sophistication (as opposed to increasing speed of convergence).

To read Sections 2–5 the student requires nothing more than familiarity with geometric series, partial fractions, and Euler's formula $e^{i\theta} = \cos\theta + i \sin\theta$. The strategy we follow in Section 5 is based on Fourier series, but we shall assume no previous exposure to this technique. Termwise integration of such series will be used, and this we will have to ask the first-year student to accept on good faith.

The examples of Sections 6 and 7 have a more advanced flavor, in that they assume some familiarity with special functions. Section 6, in which the textbook example (1) will be analyzed, requires a passing acquaintance with Bessel functions. In Section 7 we shall encounter Meijer's G-function. The author tried his best to demonstrate the peculiar convergence behavior of Section 7 using more familiar functions, but was unsuccessful. This section is therefore strictly for the aficionado.

The secondary aim of this article was to provide examples to researchers and advanced students to supplement the material in [**11**]. The authors of that paper made a commendable effort to give a characterization of the speed of convergence of the trapezoidal rule for different classes of functions, but they did not provide many examples.

The main formulas in what follows come from considering the integrals

$$I(e^{ikx}) = \int_0^{2\pi} e^{ikx}\,dx,$$

where k is an integer and $i^2 = -1$.

Suppose first that $k \neq 0$. By using the fact that $e^{2\pi ik} = 1$, we obtain

$$\int_0^{2\pi} e^{ikx}\,dx = \frac{1}{ik}e^{ikx}\bigg|_0^{2\pi} = \frac{1}{ik}\left(e^{2\pi ik} - 1\right) = 0.$$

When $k = 0$ the integral simplifies to $\int_0^{2\pi} 1\,dx = 2\pi$. We therefore conclude that

$$I(e^{ikx}) = \begin{cases} 2\pi & \text{for } k = 0, \\ 0 & \text{for } k = \pm 1, \pm 2, \dots. \end{cases} \tag{7}$$

Let us now also compute numerical approximations to these integrals. Applying the trapezoidal rule yields

$$T_N(e^{ikx}) = h\left(\tfrac{1}{2} + \sum_{j=1}^{N-1} e^{ikx_j} + \tfrac{1}{2}e^{2\pi ik}\right) = h\sum_{j=0}^{N-1} e^{2\pi ikj/N}. \tag{8}$$

The sum on the right is a finite geometric series, with common ratio $e^{2\pi ik/N}$. We can evaluate it explicitly to obtain

$$T_N(e^{ikx}) = h\frac{1 - e^{2\pi ik}}{1 - e^{2\pi ik/N}}.$$

Since k is an integer, the numerator is always zero. The denominator may also be zero: this occurs whenever k is an integer multiple of N. In the latter case, the trapezoidal sum simplifies to $T_N(e^{ikx}) = h\sum_{j=0}^{N-1} 1 = hN = 2\pi$. We infer that

$$T_N(e^{ikx}) = \begin{cases} 2\pi & \text{for } k = \ell N \quad (\ell = 0, \pm 1, \pm 2, \dots), \\ 0 & \text{otherwise.} \end{cases} \tag{9}$$

Turning to the midpoint rule, we note that

$$M_N(e^{ikx}) = e^{ikh/2}T_N(e^{ikx}). \tag{10}$$

Since $e^{ikh/2} = e^{i\pi\ell} = (-1)^\ell$ when $k = \ell N$, we conclude that

$$M_N(e^{ikx}) = \begin{cases} 2\pi(-1)^\ell & \text{for } k = \ell N \quad (\ell = 0, \pm 1, \pm 2, \ldots), \\ 0 & \text{otherwise.} \end{cases} \tag{11}$$

We are ready for our first example.

3. EXAMPLE 1 (*Perfect Convergence*). For each numerical integration rule there exists a class of functions with the property that the rule integrates all functions in this class exactly.[5] All these functions would, of course, provide examples of "faster than average" convergence.

For the trapezoidal and midpoint rules this class of functions includes the linear functions $f(x) = mx + c$. It also includes any function that is antisymmetric with respect to the line $x = \pi$, i.e., functions f for which $f(x) = -f(2\pi - x)$. For such functions both the trapezoidal and midpoint rules yield the correct value of zero.

Important special cases are the functions $\sin kx$, where k is any integer. The symmetry argument of the previous paragraph may be invoked to show that $\sin kx$ is integrated exactly for each k. Another important special case comprises the functions given for integral values of k by

$$f_1(x) = \cos kx, \qquad 0 \le x \le 2\pi.$$

If $k = 0$ the function reduces to the constant 1, which is integrated exactly, so we consider only integers $k \ge 1$. We note that $T_N(f + g) = T_N(f) + T_N(g)$. Hence

$$\cos kx = \tfrac{1}{2}\left(e^{ikx} + e^{-ikx}\right) \quad \Longrightarrow \quad T_N(f_1) = \tfrac{1}{2}\left(T_N(e^{ikx}) + T_N(e^{-ikx})\right).$$

By using the formula (9) one concludes that the exact value $I(f_1) = 0$ is obtained when k is not an integral multiple of N; in particular, this happens when $N > k$. Similar arguments apply to the midpoint rule.

On the basis of these examples one might conjecture that for a function to be in the "perfect convergence" class, symmetry is necessary. This appears not to be the case. In [**11**, p. 124] a function is cited that has no apparent symmetry properties, yet is integrated exactly by the trapezoidal rule. Involving the Möbius function of number theory, it is one of those fractal-like functions that are continuous but not absolutely continuous.

4. EXAMPLES 2 AND 3 (*Algebraic Convergence*). From perfect convergence we move to the rather slow $1/N^2$ type of convergence that is typical for both the midpoint and trapezoidal rules.

Consider

$$f_2(x) = \sin(x/2), \qquad 0 \le x \le 2\pi. \tag{12}$$

The function $\sin(x/2)$ has period 4π, not 2π. We obtain 2π-periodicity by thinking of (12) as the restriction of the function $|\sin(x/2)|$ to the interval $[0, 2\pi]$.

Proceeding as in the previous section, we observe that

$$\sin kx = \tfrac{1}{2i}\left(e^{ikx} - e^{-ikx}\right) \quad \Longrightarrow \quad T_N(f_2) = \tfrac{1}{2i}\left(T_N(e^{ikx}) - T_N(e^{-ikx})\right). \tag{13}$$

[5]We disregard, of course, the effects of roundoff error.

Each of the trapezoidal sums in parentheses is essentially a finite geometric series that we compute in a manner similar to the calculation that leads from (8) to (9). By using the fact that $e^{\pi i} = -1$, we obtain

$$T_N(e^{ix/2}) = h\left(\tfrac{1}{2} + \sum_{j=1}^{N-1} e^{ix_j/2} + \tfrac{1}{2}e^{\pi i}\right) = h\sum_{j=1}^{N-1} e^{\pi ij/N}.$$

Applying geometric series formulas to the sum on the right yields

$$\sum_{j=1}^{N-1} e^{\pi ij/N} = \frac{1+e^{\pi i/N}}{1-e^{\pi i/N}} = \frac{e^{-\pi i/(2N)} + e^{\pi i/(2N)}}{e^{-\pi i/(2N)} - e^{\pi i/(2N)}} = i\cot\frac{\pi}{2N}.$$

The trapezoidal sum $T_N(e^{-ix/2})$ can be handled similarly. We conclude that

$$T_N(e^{\pm ix/2}) = \pm hi\cot\frac{\pi}{2N}.$$

Substituting these formulas into (13), we obtain an explicit formula for the trapezoidal sum, namely,

$$T_N(f_2) = \frac{2\pi}{N}\cot\frac{\pi}{2N}.$$

We compute the true value of the integral directly as $I(f_2) = 4$ and arrive at an exact expression for the error:

$$I(f_2) - T_N(f_2) = 4 - \frac{2\pi}{N}\cot\frac{\pi}{2N}.$$

The magnitude of this error can be determined by using the Taylor expansion

$$\cot x - \frac{1}{x} = -\frac{x}{3} - \frac{x^3}{45} - \cdots, \qquad 0 < |x| < \pi \tag{14}$$

(see Abramowitz and Stegun [**1**, p. 75]). We conclude that

$$I(f_2) - T_N(f_2) \sim \frac{\pi^2}{3}\frac{1}{N^2}.$$

This estimate improves slightly on the standard estimate (3), which yields the bound $\pi^3/(6N^2)$ when $K = 1/4$. But both predict essentially a convergence rate of $1/N^2$, which is the typical situation.

Faster convergence is obtained, however, when we turn to the function

$$f_3(x) = \sin^3(x/2), \qquad 0 \le x \le 2\pi. \tag{15}$$

We again interpret this as the restriction to $[0, 2\pi]$ of the 2π-periodic function $|\sin(x/2)|^3$. (The reader may wonder why we chose to jump from the function $\sin(x/2)$ to the function $\sin^3(x/2)$, skipping the function $\sin^2(x/2)$. Well, $\sin^2(x/2) = (1-\cos x)/2$ and according to Section 3 both the trapezoidal and midpoint rules are able to integrate this exactly when $N \ge 2$.)

Using the left side of (13), here with $k = 1/2$, we compute

$$\sin^3(x/2) = \frac{i}{8}\left(e^{3ix/2} - 3e^{ix/2} + 3e^{-ix/2} - e^{-3ix/2}\right).$$

Proceeding in the same manner as earlier, we get

$$\begin{aligned} T_N(f_3) &= \frac{i}{8}\left(T_N(e^{3ix/2}) - 3T_N(e^{ix/2}) + 3T_N(e^{-ix/2}) - T_N(e^{-3ix/2})\right) \\ &= \frac{\pi}{2N}\left(3\cot\frac{\pi}{2N} - \cot\frac{3\pi}{2N}\right). \end{aligned}$$

Direct integration gives $I(f_3) = 8/3$, and an appeal to (14) shows that

$$I(f_3) - T_N(f_3) \sim -\frac{\pi^4}{30}\frac{1}{N^4}.$$

The factor $1/N^4$ confirms that the convergence is faster than typical. The standard error bound is of limited use, as the following table shows (computed with $K = 3/4$).

N	$\lvert I(f_3) - T_N(f_3)\rvert$	Error bound (3)
10	3.3×10^{-4}	1.6×10^{-1}
20	2.0×10^{-5}	3.9×10^{-2}
40	1.3×10^{-6}	9.7×10^{-3}

The reader will want to know what causes the different convergence rates in these two examples. We shall postpone such general discussions until Section 7, but for now we note that the 2π-periodic functions $\lvert\sin(x/2)\rvert$ and $\lvert\sin(x/2)\rvert^3$ have jump discontinuities in, respectively, their first and third derivatives (at $x = 0$ and $x = 2\pi$). The respective convergence rates are $1/N^2$ and $1/N^4$. The more continuous derivatives, the quicker the convergence.

To conclude this section we remark that we have focussed here on the trapezoidal rule, but explicit error formulas can also be obtained for the midpoint rule. By using the connection between the two rules summarized by (10), one deduces that each cotangent in the trapezoidal rule formulas should be replaced by the cosecant for the midpoint rule. Using the Taylor series of $\csc x - x^{-1}$ (as in [**1**, p. 75]), the asymptotic error behavior is found to be

$$I(f_2) - M_N(f_2) \sim -\frac{\pi^2}{6}\frac{1}{N^2}, \quad I(f_3) - M_N(f_3) \sim \frac{7\pi^4}{240}\frac{1}{N^4}.$$

In the next section we shall see an example of much quicker convergence.

5. EXAMPLE 4 (*Geometric Convergence*). Let a be a constant and consider

$$f_4(x) = \frac{1}{a - \cos x}, \qquad 0 \le x \le 2\pi.$$

To avoid singular integrals, we only treat the case where $a > 1$.

Like the textbook example (1), this function is 2π-periodic and smooth, and therefore one expects high accuracy. This is confirmed by the following table (computed with $a = 2$, $I(f_4) = 2\pi/\sqrt{3}$, $K = 1$).

N	$I(f_4) - M_N(f_4)$	Error bound (2)
4	3.7×10^{-2}	6.5×10^{-1}
8	1.9×10^{-4}	1.6×10^{-1}
16	5.1×10^{-9}	4.0×10^{-2}

What we intend to do is to derive an explicit formula for the errors in the middle column. This will show that the error decreases at essentially a geometric rate r^N for some positive $r < 1$ that we shall determine.

To this end, we express $f_4(x)$ as

$$f_4(x) = \frac{1}{a - (e^{ix} + e^{-ix})/2} = -2\,\frac{e^{ix}}{(e^{ix} - r)(e^{ix} - 1/r)}, \tag{16}$$

where r satisfies

$$r^2 - 2ar + 1 = 0.$$

We may choose to work with either root of this quadratic, so we pick

$$r = a - \sqrt{a^2 - 1}, \tag{17}$$

which satisfies $0 < r < 1$.

Consider the final expression in (16) as a rational function in the variable $z = e^{ix}$, and expand it in partial fractions

$$f_4(x) = 2\,\frac{r}{r^2 - 1}\left[\frac{1}{1 - re^{ix}} + \frac{1}{1 - re^{-ix}} - 1\right].$$

Since $|re^{\pm ix}| = |r| < 1$ for each real value of x, the first two terms inside the square brackets may be expanded as geometric series

$$\frac{1}{1 - re^{\pm ix}} = \sum_{k=0}^{\infty} r^k e^{\pm ikx}.$$

Finally, we obtain

$$f_4(x) = 2\,\frac{r}{1 - r^2}\left[1 + \sum_{k=1}^{\infty} r^k e^{ikx} + \sum_{k=1}^{\infty} r^k e^{-ikx}\right]. \tag{18}$$

Students who have had a course in advanced calculus or analysis will recognize in the right-hand side of (18) the Fourier series of the function $f_4(x)$.[6] We shall not make any use of the properties of Fourier series, except to note that it is in fact valid to integrate this particular series termwise with respect to x. Doing so yields, as an

[6]The function $f_4(x)$ is related to the Poisson kernel that appears in the solution of boundary value problems defined on the circle.

unexpected payoff, the exact value of the integral, namely,

$$\int_0^{2\pi} f_4(x)\,dx = 4\pi \frac{r}{1-r^2} \qquad (r = a - \sqrt{a^2-1}), \tag{19}$$

where we have used (7).

One may likewise apply the midpoint formula (11) termwise to (18) to obtain

$$M_N(f_4) = 4\pi \frac{r}{1-r^2}\left[1 + 2\sum_{\ell=1}^{\infty}(-1)^{\ell} r^{\ell N}\right].$$

Subtracting this expression from (19) yields an explicit formula for the error

$$I(f_4) - M_N(f_4) = -8\pi \frac{r}{1-r^2}\sum_{\ell=1}^{\infty}(-1)^{\ell} r^{\ell N} = 8\pi \frac{r}{1-r^2}\frac{r^N}{1+r^N}. \tag{20}$$

The formula for the trapezoidal rule is similar, except for the factor $(-1)^{\ell}$, i.e.,

$$I(f_4) - T_N(f_4) = -8\pi \frac{r}{1-r^2}\frac{r^N}{1-r^N}. \tag{21}$$

A similar result was obtained in [**5**], but there the authors used complex contour integration in their derivation.

For large N we may use the approximation $1 \pm r^N \sim 1$ to conclude that both the midpoint and the trapezoidal rule converge at essentially the exponential rate r^N. The smaller r (or the larger a), the quicker the convergence.

When $a \gg 1$ (respectively, $a \approx 1$) the integral assumes small (respectively, large) values and it is more meaningful to look at the relative (or percentage) error, which is

$$\frac{|I(f_4) - M_N(f_4)|}{|I(f_4)|} = 2\frac{r^N}{1+r^N}.$$

The relative error and the number d of correct significant digits are roughly related by [**2**, p. 18]

$$2\frac{r^N}{1+r^N} \approx \frac{1}{2} \times 10^{-d}.$$

For large N this yields

$$d \approx (-\log_{10} r)N.$$

By doubling N the number of correct significant digits approximately doubles, which affirms the quick convergence.

6. EXAMPLE 5 (*Super-geometric Convergence*). Here we increase the required background a notch, by requiring some familiarity with Bessel functions.

Let a be a positive constant, and consider the function

$$f_5(x) = e^{a\cos x}, \qquad 0 \le x \le 2\pi.$$

It includes the textbook example (1) as a special case.

We may also represent this function as a series of the form (18). Our point of departure is the generating formula for the modified Bessel functions of the first kind, $I_n(x)$, defined in [**1**, p. 376] by

$$e^{x(t+t^{-1})/2} = \sum_{k=-\infty}^{\infty} I_k(x)t^k.$$

From the substitutions $x \mapsto a$ and $t \mapsto e^{ix}$ follows

$$e^{a\cos x} = I_0(a) + \sum_{k=1}^{\infty} I_k(a)e^{ikx} + \sum_{k=1}^{\infty} I_k(a)e^{-ikx}. \tag{22}$$

We have used the fact that $I_k(x) = I_{-k}(x)$, $k = 1, 2, \ldots$.

Integrating term-by-term yields the true value of the integral as[7]

$$\int_0^{2\pi} e^{a\cos x}\, dx = 2\pi I_0(a). \tag{23}$$

Summing (22) term-by-term yields the midpoint approximation to this integral as

$$M_N(f_5) = 2\pi I_0(a) + 4\pi \sum_{\ell=1}^{\infty}(-1)^{\ell} I_{\ell N}(a),$$

for which the error is

$$I(f_5) - M_N(f_5) = -4\pi \sum_{\ell=1}^{\infty}(-1)^{\ell} I_{\ell N}(a). \tag{24}$$

The error formula for the trapezoidal rule is identical except for the factor $(-1)^{\ell}$.

The Bessel functions $I_k(x)$ decay rapidly for fixed x as $k \to \infty$; namely, from [**1**, pp. 365 and 375] we learn that

$$I_k(x) \sim \frac{1}{\sqrt{2\pi k}} \left(\frac{ex}{2k}\right)^k.$$

This means that we may retain only the first term in (24), i.e.,

$$\begin{aligned} I(f_5) - M_N(f_5) &\sim 4\pi I_N(a) \\ &\sim 2\left(\frac{2\pi}{N}\right)^{1/2}\left(\frac{ea}{2N}\right)^N, \end{aligned}$$

which is how we arrived at the estimate (6).

The convergence rate is essentially of the form r^N, with $r = (ea)/(2N)$. Since $r \to 0$ as $N \to \infty$, the convergence rate is often referred to as super-geometric (see Boyd [**3**, p. 32]).

7. EXAMPLE 6 (*Sub-geometric Convergence*). Mainly of academic interest, our final example assumes particular knowledge of Fourier series and special functions.

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[7]The result (23) is not to be sneered at. Only one of the three CASs we tried was able to carry out this integration in symbolic form, even when we put $a = 1$.

Consider

$$f_6(x) = \begin{cases} e^{(\cos x - 1)/(\cos x + 1)} & 0 \le x \le 2\pi,\ x \ne \pi, \\ 0 & x = \pi. \end{cases} \tag{25}$$

This function is 2π-periodic and, as can be checked without great difficulty, is infinitely differentiable. High accuracy is to be expected when its integral is approximated by the trapezoidal or midpoint rules, and that this is indeed the case may be seen in the table following relation (30). (To compute the error, we have used a CAS to establish that $I(f_6) = 2e\pi(1 - \operatorname{erf} 1) = 2.68658684\ldots$, where erf is the error function defined in [**1**, p. 297].)

An explicit formula for the error may be derived by assuming a Fourier series expansion of the form

$$f_6(x) = \sum_{k=-\infty}^{\infty} c_k e^{ikx}, \tag{26}$$

where the Fourier coefficients are given by

$$c_k = \frac{1}{2\pi} \int_0^{2\pi} f(x) e^{-ikx}\, dx. \tag{27}$$

Through repeated integration by parts, it can be deduced from (27) that the Fourier coefficients satisfy $c_k = O(|k|^{-\ell})$ for each integer ℓ.

Integrating and then summing both sides of (26) leads to

$$I(f_6) = 2\pi c_0, \qquad T_N(f_6) = 2\pi c_0 + 2\pi \sum_{\substack{\ell=-\infty \\ \ell \ne 0}}^{\infty} c_{\ell N},$$

where we have used (7) and (9). The error is

$$I(f_6) - T_N(f_6) = -2\pi \sum_{\substack{\ell=-\infty \\ \ell \ne 0}}^{\infty} c_{\ell N}. \tag{28}$$

The midpoint error is similar, except for the usual $(-1)^\ell$ factor.

The Fourier coefficients of the function $f_6(x)$ can in fact be computed explicitly in terms of Meijer's G-function. We omit the details but refer the reader to [**15**, p. 1501] and [**16**, pp. 125–126]. The result is

$$c_k = \frac{e}{\sqrt{\pi}} G^{30}_{23}\left(1 \middle| \begin{array}{ccc} 1-k, & & 1+k \\ 1, & \frac{1}{2}, & 0 \end{array}\right), \quad k = 0, \pm 1, \pm 2, \ldots.$$

Since these coefficients decay quite rapidly (recall the remark that follows (27)), we retain only the two terms corresponding to $\ell = \pm 1$ in (28) to estimate the error as[8]

$$I(f_6) - T_N(f_6) \sim -4\, e \sqrt{\pi}\, G^{30}_{23}\left(1 \middle| \begin{array}{ccc} 1-N, & & 1+N \\ 1, & \frac{1}{2}, & 0 \end{array}\right). \tag{29}$$

An asymptotic estimate of the function on the right has been carried out by the author in [**15**, pp. 1501–1510], and the result is

[8]The G-function in the error estimate (29) may be computed in Maple by

```
MeijerG([ ], [ ], [1-N, 1+N], [1, 1/2, 0], [ ], 0).
```

$$I(f_6) - T_N(f_6) \sim (-1)^{N+1} 8(\pi/3)^{1/2} e^{2/3} N^{-2/3}$$
$$\times \cos\left(\tfrac{3^{3/2}}{2} N^{2/3} + \tfrac{\pi}{3}\right) \exp\left(-\tfrac{3}{2} N^{2/3}\right). \qquad (30)$$

These estimates are sharp, even for relatively small N:

N	$\lvert I(f) - T_N(f)\rvert$	|Estimate (29)|	|Estimate (30)|
10	2.8×10^{-3}	2.8×10^{-3}	2.8×10^{-3}
20	7.7×10^{-6}	7.6×10^{-6}	7.8×10^{-6}
40	3.3×10^{-8}	3.3×10^{-8}	3.3×10^{-8}

The speed of convergence is essentially determined by the exponential term $e^{-(3/2)N^{2/3}}$ in (30). It indicates a convergence rate quicker than the algebraic convergence of Section 4, but not quite as fast as the geometric convergence of Section 5. This is often referred to as sub-geometric convergence (see Boyd [**3**, p. 32]).

Note also the oscillatory cosine term in (30). It may assume values close to zero, which would imply high accuracy. The zeros of the cosine term occur where

$$N = \left[\frac{2\pi}{3^{3/2}}\left(\frac{6k-5}{6}\right)\right]^{3/2}, \quad k = 1, 2, 3, \ldots.$$

By taking the nearest integer one obtains a sequence of values, namely,

$$N = 2, 4, 7, 11, 16, 20, 26, 31, 37, 43, 50, 56, 64, 71, 79, \ldots,$$

that should yield particularly small errors. For example, with $N = 31$ one gets $I(f_6) - T_{31}(f_6) \approx 7.5 \times 10^{-9}$. Increasing the number of subintervals to $N = 33$ yields the significantly larger error $I(f_6) - T_{33}(f_6) \approx -2.7 \times 10^{-7}$. The author knows of no other class of functions that exhibits this nonmonotonic pattern of convergence.

8. GENERAL ERROR FORMULAS. The examples presented in the previous sections were special in that we were able to derive, in most cases, explicit formulas for the error.[9] For general integrals the best one could hope to do is estimate the error. To learn more about such error estimates the student is encouraged to consult the literature (for example [**2**], [**7**], or [**9**]).

One of those references, Gautschi [**7**, p. 155], uses the Fourier series as basis for a convergence analysis of the trapezoidal rule. This is essentially the approach we followed in Sections 5–7. When the Fourier coefficients decay to zero quickly, as they do for functions $f_4(x)$, $f_5(x)$, and $f_6(x)$, then the formula (28) provides a good estimate for the error. On the other hand, when the c_k approaches zero only algebraically, like $1/|k|^\ell$, then (28) should not be used as it stands. To see why not, consider for example the function $f(x) = e^{-x}$ defined on $[0, 2\pi]$. Its Fourier coefficients are $c_k = (1/2\pi)(1 - e^{-2\pi})/(1 + k\,i)$, which decay like $1/k$. As a result, the series in (28) does not converge. Yet both the midpoint and trapezoidal rule approximations converge according to the standard $1/N^2$. (The situation can be remedied by considering only the cosine-part of the Fourier expansion, as in [**7**, p. 155].)

An alternative for functions of relatively low continuity is the Euler-Maclaurin summation formula, which we state here for a function $f(x)$ that is not necessarily periodic. The proof may be found in Atkinson [**2**, p. 285].

[9] If one thinks about it, an explicit formula for the error means one can obtain the value of the integral exactly, and numerical integration would not be necessary in the first place!

Theorem 1. *Let $m \geq 0$, $N \geq 1$, and define $h = 2\pi/N$, $x_j = jh$ for $j = 0, 1, \ldots, N$. Further assume that $f(x)$ is $2m+2$ times continuously differentiable on $[0, 2\pi]$ for some $m \geq 0$. Then, for the error in the trapezoidal rule defined by (3),*

$$I(f) - T_N(f) = -\sum_{k=1}^{m} \frac{B_{2k}}{(2k)!} h^{2k} \left[f^{(2k-1)}(2\pi) - f^{(2k-1)}(0) \right] \qquad (31)$$

$$- 2\pi h^{2m+2} \frac{B_{2m+2}}{(2m+2)!} f^{(2m+2)}(\xi)$$

*for some ξ in $[0, 2\pi]$. The B_k are the Bernoulli numbers [**1**, p. 804].*

The typical case corresponds to $m = 0$, in which the sum in (31) is void. Using the fact that $B_2 = 1/6$, the formula reduces to

$$I(f) - T_N(f) = -h^2 \frac{\pi}{6} f^{(2)}(\xi),$$

which leads to the standard error bound (3). Note, however, that if the odd derivatives of $f(x)$ at $x = 0$ and at $x = 2\pi$ are equal, the terms in the sum in (31) cancel, and the convergence may be quicker than usual.

This was the situation for the function $f_3(x) = \sin^3(x/2)$. Since $f_3'(0) = f_3'(2\pi)$, but $f_3'''(0) \neq f_3'''(2\pi)$, one may take $m = 1$ in the Euler-Maclaurin formula, which then predicts a convergence rate of order h^4 or $1/N^4$. By contrast, the function $f_2(x) = \sin(x/2)$ does not have equal first derivatives at the endpoints of the interval $[0, 2\pi]$, and the regular convergence rate of $1/N^2$ is obtained.

The Euler-Maclaurin formula raises the interesting possibility of certain functions posing as "pseudo-periodic" functions, at least in finite precision arithmetic. Consider, for example, the nonperiodic function

$$f_7(x) = e^{-x^2}, \qquad 0 \leq x \leq 2\pi. \qquad (32)$$

Approximations by the trapezoidal rule yield the errors listed in the following table (once again in comparison with the standard error bound (3), with $K = 2$):

N	$\lvert I(f) - T_N(f_7)\rvert$	Error bound (3)
6	2.2×10^{-4}	1.1×10^{0}
8	2.0×10^{-7}	6.5×10^{-1}
10	2.5×10^{-11}	4.1×10^{-1}

The function (32) does not satisfy $f_7'(0) = f_7'(2\pi)$, and therefore one expects the typical convergence rate $1/N^2$. The numerical results in the table, however, seem to indicate much quicker convergence. To see why, note that all odd derivatives at $x = 0$ vanish, while at $x = 2\pi$ many of them are negligible: $f_7'(2\pi) \approx 10^{-16}$, $f_7'''(2\pi) \approx 10^{-14}$, $f_7'''''(2\pi) \approx 10^{-12}$, etc. When working to about sixteen significant digits, as we did here, the derivative terms in the Euler-Maclaurin formula cancel for all practical purposes and the numerical results indicate a convergence rate much faster than the expected $1/N^2$. It should be kept in mind, however, that the numbers in the middle column represent transient behavior. If the computations were done to higher precision and for larger values of N, the convergence would eventually settle into the standard $1/N^2$ rate.

The argument of the previous paragraph shows why spectacular accuracy may be achieved when the trapezoidal rule is applied to integrals of the form

$$I = \int_{-\infty}^{\infty} e^{-x^2} f(x)\,dx.$$

This observation dates back at least half a century to a paper of E.T. Goodwin [**8**], which was inspired by a paper of Alan Turing [**10**, p. 214]. In turn, these developments inspired Frank Stenger to develop the powerful machinery of sinc functions [**12**].

For periodic functions that are infinitely differentiable, like our functions $f_4(x)$, $f_5(x)$, and $f_6(x)$, the Euler-Maclaurin formula predicts a convergence rate faster than any power of h (or $1/N$). On the other hand, the formula is not sufficiently powerful to determine the rate precisely. For this one has to go to methods based on analytic function theory. Using residue calculus, for example, the following theorem may be proved [**9**, p. 211].

Theorem 2. *Let $f : \mathbb{R} \longrightarrow \mathbb{R}$ be analytic and 2π-periodic. Then there exists a strip $D = \mathbb{R} \times (-c, c) \subset \mathbb{C}$ with $c > 0$ such that f can be extended to a bounded holomorphic and 2π-periodic function $f : D \longrightarrow \mathbb{C}$. The error for the trapezoidal rule can be estimated by*

$$|I(f) - T_N(f)| \leq 4\pi \frac{M}{e^{cN} - 1}, \tag{33}$$

where M denotes a bound for the holomorphic function f on D.

This theorem says that if the 2π-periodic function $f(z)$ is analytic in a strip $|\mathrm{Im}(z)| < c$, then geometric convergence of the form r^N, with $r = e^{-c} < 1$, is assured. The wider the strip of analyticity, the quicker the convergence.

The functions of Sections 5 and 6 are in this class. Consider $f_4(z) = 1/(a - \cos z)$, $a > 1$, which has simple poles at points where $\cos z = a$, i.e., at

$$z_k = 2k\pi \pm \gamma i, \qquad k = 0, \pm 1, \pm 2, \ldots,$$

with $\gamma = \log(a + \sqrt{a^2 - 1})$. The strip of analyticity is therefore determined by $c < \gamma$. This means that the convergence rate is essentially of the form $e^{-cN} = 1/(a + \sqrt{a^2 - 1})^N = (a - \sqrt{a^2 - 1})^N$, which is consistent with our exact expression for the error (see (21)).

The textbook function $f(z) = e^{\cos z}$ is entire; i.e., it has no singularities in the finite complex plane. One cannot take the strip $|\mathrm{Im}(z)| < c$ infinitely wide, however, as M grows unboundedly as $c \to \infty$. In fact, a quick calculation shows that the least upper bound for $f(z)$ in the strip $|\mathrm{Im}(z)| < c$ is $M = e^{\cosh c}$, and substitution into (33) yields

$$|I(f) - T_N(f)| \leq 4\pi \frac{e^{\cosh c}}{e^{cN} - 1}.$$

A minimization argument shows that to make the right-hand side a tight bound for each (large) value of N, a choice like $c = \sinh^{-1} N$ or $\cosh^{-1} N$ should be made. Choosing the latter gives

$$|I(f) - T_N(f)| \leq 4\pi \frac{e^N}{e^{N\cosh^{-1} N} - 1}.$$

As $N \to \infty$ the bound on the right decreases like $4\pi(e/2N)^N$. Aside from a factor $\sqrt{2\pi N}$, this is identical to the super-geometric convergence defined by (6).

The function $f_6(x)$ studied in Section 7 was a pathological case squeezed between Theorems 1 and 2 (and that is why we chose to include it). Since $f_6(x)$ is infinitely differentiable on $[0, 2\pi]$, the Euler-Maclaurin formula predicts a convergence rate more rapid than $1/N^\ell$ for any $\ell > 0$. However, because this function has an essential singularity at $x = \pi$, it is not analytic in any strip $|\mathrm{Im}(z)| < c$ with $c > 0$. This means that the error estimate (33) cannot be applied to this situation to establish geometric convergence. Indeed, the convergence rate of $e^{-(3/2)N^{2/3}}$ derived in Section 6 falls somewhere between algebraic and geometric convergence.

Perhaps the most comprehensive attempt at classifying the speed of convergence of the trapezoidal rule was given by Rahman and Schmeisser in [**11**]. They made a convincing point that functions can be catalogued into different smoothness classes on the basis of the speed of convergence of the trapezoidal rule.

9. CONCLUSIONS. The main theme of this essay is that, when the integrand is smooth and periodic, the midpoint and trapezoidal rules are very efficient. Using more sophisticated rules may not be worth the effort. One such rule is Simpson's rule, which normally converges at a rate $1/N^4$. Typically derived by computing the area under piecewise quadratic approximations of the function, Simpson's rule may also be viewed as a weighted average of the midpoint and trapezoidal rules

$$S_N(f) = \tfrac{2}{3}M_{N/2}(f) + \tfrac{1}{3}T_{N/2}(f).$$

When this rule is applied to the function $f_4(x) = 1/(a - \cos x)$, for example, the error estimates (20) and (21) show that the rate of convergence is roughly $r^{N/2}$ (with r defined by (17)). This is faster convergence than the $1/N^4$ rate that is typical for Simpson's rule. Nevertheless, one would need about twice as many points to achieve the same accuracy as either the midpoint or the trapezoidal rule.

One should not conclude from this, however, that the midpoint or the trapezoidal rule beat all-comers hands down when the integrand is smooth and periodic. For $f_4(x) = 1/(a - \cos x)$, with $a = 1 + \epsilon$ and $0 < \epsilon \ll 1$, the powerful Gauss-Legendre rule is superior, although this superiority disappears as a increases (see Davis [**4**, p. 54]). If one changes the minus sign in the denominator into a plus (so that the peak of the graph is in the middle of the interval rather than at the endpoints), then the midpoint and trapezoidal rules remain the clear winners, as demonstrated in [**5**]. Numerical results have also indicated that both the midpoint and trapezoidal rules integrate the functions $f_5(x)$ and $f_6(x)$ better than the Gauss-Legendre rule does.

The rapid speed of convergence may be exploited in various ways. First, it may be useful for the computation of special functions (see Luke [**10**, chapter 15]). The application of these rules to the integral (23), for instance, represents a respectable tool for computing $I_0(x)$, provided x is not too large.

Second, consider an integral for which the typical rate of convergence is the standard $1/N^2$. One may attempt to improve the accuracy by a change of variables, with the aim of making the integrand "more periodic." Such transformation methods are discussed in [**6**, pp. 107–135] and [**9**, p. 220].

Third, there is the Fourier spectral method. Based on the differentiation of truncated Fourier series such as (26), this is a powerful method for solving differential equations [**3**], [**14**]. When the underlying function is smooth and periodic, the rate of convergence of the Fourier spectral method is similar to the rate of convergence of the trapezoidal/midpoint rules. Indeed, several of our examples can be used to quantify the convergence curves of the spectral method displayed in [**14**, p. 36].

Fourth, and perhaps most importantly, is the computation of Fourier coefficients. Applying the trapezoidal rule to the integral (27) and assuming $f(0) = f(2\pi)$ yields

$$c_k \approx \frac{1}{N} \sum_{j=0}^{N-1} f(x_j) e^{2\pi ijk/N}.$$

Not only has our discussion shown that this is the "right" way to approximate the integral, but the sum may be evaluated efficiently with the Fast Fourier Transform (see Atkinson [**2**, p. 181] or Kress [**9**, p. 167]). This is an algorithm that approximates N of the coefficients c_k in asymptotically $O(N \log N)$ algebraic operations. By contrast, direct summation requires $O(N^2)$ operations. The FFT has revolutionized approaches to applications such as signal processing and digital imaging.

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