Basic Numerical Analysis*

Jonathan Goodman

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1 Introduction

The most basic technique in numerical analysis is manipulation of Taylor series expansions. This is how we find numerical methods for differentiation and integration, for solving differential equations, for optimization, and for many other purposes. The same kind of analysis leads to quantitative understanding of the error in many numerical approximations. These "asymptotic error expansions" are used for validating complex numerical software and for developing efficient adaptive computational algorithms.

We will be concerned with efficiency. Here, efficiency means finding the derivative accurately using a large step size, finding an integral accurately using a small number function evaluations, etc. For casual computation such concern is probably a waste of time; more time is spent optimizing the code than could possibly be saved in a computation that takes less than a second on the computer. However, we will see that these simple operations are at the heart of algorithms that solve partial differential equations, algorithms whose running time and accuracy are of serious concern.

We will often use the phrase "for sufficiently small h" without clarifying how small is small enough. This issue is too problem dependent to settle in a simple general way. When h is small enough, we say that "h is in the asymptotic range", the range in which an asymptotic expansion gives useful information. It is often clear from the problem roughly how large the asymptotic range is likely to be, and that range is usually large enough to cover practical h values. If a code is unable to produce results consistent with an asymptotic error analysis, it is generally not because the asymptotic range is inaccessible. Look instead for a bug in the code, in the method, or in the error analysis.

The three specific problems discussed in this chapter are differentiation, integration, and interpolation. Numerical differentiation is the problem of finding (as accurately as necessary) a derivative of a function, given several values of the function itself. Numerical integration is the problem of computing the integral. Interpolation is the problem of evaluating a function at some value of its arguments given as data function values at other values of the arguments.

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Each of these topics is treated from the point view of asymptotic error expansions. The chapter also discusses asymptotic error expansions, and their uses, in general.

2 Taylor series and asymptotic expansions

The[1] Taylor series may be thought of in two ways, as a "convergent" formula for a function value, or as an "asymptotic expansion", a sequence of approximations of increasing "order of accuracy". All of these terms are explained below.

Suppose we have a function, $f(x)$, and a "step size", h. The Taylor series for f about x is

$$f(x+h) = f(x) + hf'(x) + \frac{h^2}{2}f''(x) + \cdots + \frac{h^n}{n!}f^{(n)}(x) + \cdots \quad . \tag{1}$$

The series (1) "converges" if

$$f(x) + \cdots + \frac{h^n}{n!}f^{(n)}(x) \to f(x+h) \quad \text{as } n \to \infty. \tag{2}$$

Generally speaking, if you can write a formula for $f(x)$ then the expansion will converge for sufficiently small h. The formula (2) suggests that we improve the accuracy of the Taylor series approximation by taking more terms.

The accuracy also increases if we make h smaller; it will become clear later why we are allowed to do this. One way to prove that Taylor series converge is to use the "remainder theorem", which is the formula:

$$f(x+h) - \left(f(x) + + \cdots + \frac{h^n}{n!}f^{(n)}(x) \right) = \frac{h^{(n+1)}}{(n+1)!}f^{(n+1)}(\xi) \quad . \tag{3}$$

This ξ depends on x, h, and n in an unknown way, except that ξ is between x and $x+h$. If h is negative, then $x+h$ is to the left of x, but still ξ is between. If we fix a maximum step size, h_0, and set

$$M_{n+1} = \max_{|h| \leq h_0} \left| f^{(n+1)}(x+h) \right| / (n+1)! \ , \tag{4}$$

then (3) gives us a bound on how large the Taylor series error can be. This bound is

$$\left| f(x+h) - \left(f(x) + \cdots + \frac{h^{(n-1)}}{(n-1)!}f^{(n-1)}(x) \right) \right| \leq M_n \left| h^n \right| \quad . \tag{5}$$

The inequality (5) does not guarantee that the Taylor series converges, because $M_n h^n$ need not go to zero as $n \to \infty$. However, it does say something about what happens, for any particular n, as $h \to 0$.

To summarize, we can think of (1) as a way to compute a particular value of f, in which case we keep h fixed and increase n. We could instead view (1) as a family of approximations to the function f for values near x. The error bound (5) gives a sense in which using more

[1] This section was added last. Therefore many of the points made here are repeated later.

terms gives a better approximation. If $E(h)$ is the error on the left side of (5), then (5) is often written

$$E(h) = O(h^n) \ . \tag{6}$$

This is called the "big O" notation. A mathematician would read (6) as "$E(h)$ is of the order of h^n. This is what we think of as an order of magnitude, not a power of 10 but a power of h. The power of h is the "order of accuracy", first order, second order, and so on.

Very often we use Taylor series as asymptotic series to understand the asymptotic accuracy, or the order of accuracy, of simple approximations. We also use them to find asymptotic approximations for the error itself. For example, if we approximate $f(x+h)$ using two terms of the Taylor expansion, the error is

$$E(h) = f(x+h) - f(x) - hf'(x) \ .$$

The approximation is second order accurate because $E(h) \leq Mh^2$, for some constant, M, if h is small enough. However, we can say more about the error. In fact, if we just keep more terms of the Taylor series, we find that

$$E(h) \approx a_3 h^3 + a_4 h^4 + \cdots \ , \tag{7}$$

where the coefficients a_3, a_4, and so on are determined by f. For example, the statement $E(h) \leq Mh^2$ does not necessarily imply that the error decreases when we substitute $h/2$ for h, although it does imply that the error eventually goes down so as not to exceed the error bound. On the other hand, (7) implies that, for sufficiently small h, the error goes down almost exactly by a factor of 8. This predictability of the error in approximations is the basis for much sophisticated numerical software.

As the formula (4) indicates, all this asymptotic expansion stuff might not apply if the function does not have enough derivatives. This can happen even with functions that seem nice enough when you plot them. It is hard to tell from a plot where, for example, the third derivative is discontinuous. A discontinuity in the third derivative can invalidate the asymptotic expansions that predict order of accuracy and change the behavior of the error sometimes disastrous ways.

3 Numerical Differentiation

We start with the simplest case. Suppose we have a smooth function, $f(x)$, of a single variable, x. If we can evaluate f but not $f' = \frac{df}{dx}$, we could approximate f' by a difference quotient. Several common approximations are

$$\left.\begin{aligned}
f'(x) &\approx \frac{f(x+h)-f(x)}{h} && (a)\\
f'(x) &\approx \frac{f(x)-f(x-h)}{h} && (b)\\
f'(x) &\approx \frac{f(x+h)-f(x-h)}{2h} && (c)\\
f'(x) &\approx \frac{-f(x+2h)+4f(x+h)-3f(x)}{2h} && (d)\\
f'(x) &\approx \frac{-f(x+2h)+8f(x+h)-8f(x-h)+f(x+2h)}{12h} && (e)
\end{aligned}\right\} \qquad (8)$$

The first three have simple geometric interpretations as the slope of lines connecting nearby points on the graph of $f(x)$. A carefully drawn figure shows that (8c) is more accurate than (8a). We give an analytical explanation of this below. The last two are more technical.

The advantage of the last one over the others is its greater accuracy. If h is small enough, the error in (8e) is likely to be much less than the error in the others. This often (but not always) has the consequence that (8e) achieves a given level of accuracy (say 1%) for a larger h value, a property that leads to greater efficiency when solving differential equations.

To perform a basic error analysis, we use the Taylor series expansion (1). Substituting this into (8a) gives

$$\frac{f(x+h)-f(x)}{h} = f'(x) + h\frac{f''(x)}{2} + h^2\frac{f'''(x)}{6} + \cdots \ .$$

Now we can express the error in formula (8a) by:

$$f'(x) = \frac{f(x+h)-f(x)}{h} + E_a(h) \ ,$$

where

$$E_a(h) = \frac{h}{2}f''(x) + \frac{h^2}{6}f'''(x) + \cdots \ . \qquad (9)$$

If h is small, then h^2 is smaller still; h^2 is smaller than h by a factor of h. Thus, $\frac{h^2}{6}f'''(x)$ will be much smaller than $\frac{h}{2}f''(x)$ unless $f'''(x)$ is much larger than $f''(x)$. When h is small enough, we may approximate the error by

$$E_a(h) \approx \frac{h}{2}f''(x) \ .$$

This tells the story about approximation (8a). The error depends roughly linearly on h (for small enough h). Cutting h in half reduces the error roughly in half. The same is true of the related approximation (8b). The approximations (8a) and (8b) are called "first order one sided difference approximations" to the derivative.

Taylor series analysis applied to the centered difference approximation (8c) leads to

$$f'(x) = \frac{f(x+h) - f(x-h)}{2h} + E_c(h)$$

where

$$\begin{aligned} E_c(h) &= \frac{h^2}{6} f'''(x) + \frac{h^4}{24} f^{(5)}(x) + \cdots \\ &\approx \frac{h^2}{6} f'''(x) \quad \text{for } h \text{ small enough.} \end{aligned} \tag{10}$$

In this case, the error depends quadratically on h instead of linearly. Moreover the error from (8c) is much smaller than the error from (8a) or (8b). That is[2],

$$\frac{h^2}{3} f'''(x) \ll \frac{h}{2} f''(x) \quad \text{i.e.} \quad E_c(h) \ll E_a(h) \text{ for small enough } h.$$

When the error is on the order of h for small h we say that the approximation is first order accurate. When it is of the order of h^2 we call it second order accurate, and similarly for third, fourth, and higher powers of h. A Taylor series analysis shows that (8d) is second order accurate while (8e) is fourth order. If h is small and the derivatives of f up to fifth order are not extremely large then (8c) and (8d) are more accurate than (8a) or (8b), and (8e) is more accurate than any of the others. The approximation (8c) is called the "second order three point centered difference approximation" to the derivative; (8d) is the "three point one sided second order" difference approximation; (8e) is the "five point centered fourth order" approximation.

As mentioned before, a difference approximation may not achieve its expected order of accuracy if the requisite derivatives are infinite or do not exist. As an example of this, let $f(x)$ be the function

$$f(x) = \begin{cases} 0 & \text{if } x \leq 0 \\ x^2 & \text{if } x \geq 0 \end{cases} .$$

If we want $f'(0)$, the formulas (1c) and (1e) are only first order accurate despite their higher accuracy for smoother functions. This f has a mild singularity, a discontinuity in its second derivative. Such a singularity is hard to spot on a graph. Nevertheless, it has a drastic effect on the numerical analysis of the function.

We can use finite differences to approximate higher derivatives such as

$$f''(x) = \frac{f(x+h) - 2f(x) + f(x-h)}{h^2} + \frac{h^2}{12} f^{(4)} + \cdots ,$$

and to estimate partial derivatives of functions depending on several variables, such as

$$\frac{\partial}{\partial x} f(x,y) = \frac{f(x+h,y) - f(x-h,y)}{2h} + \frac{h^2}{3} \frac{\partial^3 f}{\partial x^3}(x,y) + \cdots .$$

[2]The notation $A \ll B$ is read "A is much smaller than B".

We can approximate sums of partial derivatives by adding the separate difference approximations. For example

$$\triangle f = \frac{\partial^2 f}{\partial x^2} + \frac{\partial^2 f}{\partial y^2} \approx \frac{f(x+h,y) + f(x-h,y) + f(x,y+h) + f(x,y-h) - 4f(x,y)}{h^2} \quad .$$

This is called "the standard 5 point discrete Laplacian". It is not necessary to approximate $\triangle f$ by approximating the second partials separately in this way. Another second order accurate approximation is

$$\triangle f(x,y) \approx \frac{f(x+h,y+h) + f(x+h,y-h) + f(x-h,y+h) + f(x-h,y-h) - 4f(x,y)}{2h^2} \quad .$$

This "rotated 5 point" approximation is rarely preferable to the standard, one.

A multidimensional complication is that we might use different step sizes in different coordinate directions. An important example of this arises when we compute a function, $f(x,t)$ that satisfies a partial differential equation such as

$$\frac{\partial f}{\partial t} = \frac{\partial^2 f}{\partial x^2} \quad .$$

To evaluate the combination

$$\frac{\partial f}{\partial t} - \frac{\partial^2 f}{\partial x^2} \quad , \tag{11}$$

we need a "time step", Δt, and a "space step", Δx. For example, we might use

$$\frac{\partial f}{\partial t} \approx \frac{f(x, t + \Delta t) - f(x,t)}{\Delta t} \tag{12}$$

and

$$\frac{\partial^2 f}{\partial x^2} \approx \frac{f(x + \Delta x, t) - 2f(x,t) + f(x - \Delta x, t)}{2\Delta x} \quad . \tag{13}$$

The approximation (12) has error roughly $\Delta t \frac{\partial^2 f}{\partial t^2}/2$ which is first order in Δt. The approximation (13) has error roughly $\Delta x^2 \frac{\partial^4 f}{\partial x^4}/6$, which is second order in Δx. If we now take $\Delta x = h$ and $\Delta t = h^2$ then the principle term in the error in the approximation to (11) is is

$$h^2 \left(\frac{1}{2} \frac{\partial^2 f}{\partial t^2} + \frac{1}{6} \frac{\partial^4 f}{\partial x^4} \right) \quad .$$

This example illustrates the point that the overall order of accuracy depends not only on the order of accuracy of the individual approximations, but also on the choice of step sizes in various directions.

4 Error Expansions and Richardson Extrapolation

The error expansions (9) and (10) above are instances of a common situation that we now describe more systematically and abstractly. Suppose we are trying to compute a number,

A, which is the "Answer" to some computational problem. We have an approximation to A that depends on a step size, h:

$$A \approx A(h) \ .$$

The approximation becomes increasingly accurate as h becomes small:

$$A(h) \to A \ \text{ as } \ h \to 0 \ .$$

The error is $E(h) = A(h) - A$.

An "asymptotic error expansion" in powers of h can be expressed either by

$$A(h) \approx A + h^{p_1} A_1 + h^{p_2} A_2 + \cdots \quad , \tag{14}$$

or, equivalently, by

$$E(h) \approx h^{p_1} A_1 + h^{p_2} A_2 + \cdots \quad .$$

The expression (14) does not imply that the series on the right converges to $A(h)$, but rather it is a substitute for the statements that make it an asymptotic series:

$$\left.\begin{array}{lll} \dfrac{A(h) - (A + h^{p_1} A_1)}{h^{p_1}} \to 0 & \text{as } h \to 0, & (a) \\[2ex] \dfrac{A(h) - (A + h^{p_1} A_1 + h^{p_2} A_2)}{h^{p_2}} \to 0 & \text{as } h \to 0, & (b) \\[2ex] \text{and so on.} & & \vdots \end{array}\right\} \tag{15}$$

The statement (15a) says not only that $A + h^{p_1}$ is a good approximation to $A(h)$, but that the error in the approximation is smaller than h^{p_1} for small enough h. The statement (15b) says that $A + h^{p_1} A_1 + h^{p_2} A_2$ is a better approximation to $A(h)$ in that the error is smaller than h^{p_2}, which is much smaller than h^{p_1} for small h. It goes without saying that $0 < p_1 < p_2 < \cdots$. In many cases, the powers and coefficients are found by Taylor series manipulations. For the approximations (8a) and (8b), $p_1 = 1$, $p_2 = 2$, $p_3 = 3$, and so on. For (8c), $p_1 = 2$, $p_2 = 4$, $p_3 = 6$, and so on. Although (8d) has the same order as (8c), $p_1 = 2$ in both cases, but its asymptotic error expansion, $p_2 = 3$, $p_3 = 4$, etc. is different (work this out!). In all cases the principal error term is dominant when h is small enough. How small is small enough depends on the coefficients, A_1, A_2, etc. The leading power, p_1, determines the order of accuracy, as we have seen. This order need not be an integer. Methods with fractional order of accuracy sometimes arise, particularly in simulation of stochastic differential equations. Two methods may have the same order of accuracy but different asymptotic error expansions, as we have seen.

It is possible that an approximation is pth order accurate in the "big O" sense, $E(h) = O(h^p)$, without having an asymptotic error expansion of the form (14). An example of this is coming.

It can be valuable to know the *existence* of an error expansion of the form (14) even if the coefficients, A_1, A_2, ..., cannot be determined. The two main applications are **convergence analysis** and **Richardson extrapolation**. In convergence analysis, we verify empirically

h	Error: $E(h)$	Ratio: $E(h)/E(h/2)$
.1	4.8756e-04	3.7339e+00
.05	1.3058e-04	6.4103e+00
.025	2.0370e-05	7.3018e+00
.0125	2.7898e-06	7.6717e+00
6.2500e-03	3.6364e-07	7.8407e+00
3.1250e-03	4.6379e-08	7.9215e+00
1.5625e-03	5.8547e-09	7.9611e+00
7.8125e-04	7.3542e-10	———-

Figure 1: Convergence Study for a third order accurate approximation

h	Error: $E(h)$	Ratio: $E(h)/E(h/2)$
.1	1.9041e-02	2.4014e+00
.05	7.9289e-03	1.4958e+01
.025	5.3008e-04	-1.5112e+00
.0125	-3.5075e-04	3.0145e+00
6.2500e-03	-1.1635e-04	1.9880e+01
3.1250e-03	-5.8529e-06	-8.9173e-01
1.5625e-03	6.5635e-06	2.8250e+00
7.8125e-04	2.3233e-06	———-

Figure 2: Convergence Study for a method that has no asymptotic expansion

the supposed order of accuracy of numbers produced by a computer code that may be large, unknown, and contain bugs. In Richardson extrapolation, we combine approximations for several values of h to produce a new approximation that has greater order of accuracy than $A(h)$.

4.1 Richardson extrapolation

Richardson extrapolation is a method that increases the order of accuracy of an approximation provided that the approximation has an asymptotic error expansion of the form (14). In its simplest form, we compute $A(h)$ and $A(2h)$ and then form a linear combination that eliminates the largest error term, $h^{p_1}A_1$. Since

$$\begin{aligned} A(2h) &= A + (2h)^{p_1} A_1 + (2h)^{p_2} A_2 + \cdots \\ &= A + 2^{p_1} h^{p_1} A_1 + 2^{p_2} h^{p_2} A_2 + \cdots \quad , \end{aligned}$$

we find that

$$\frac{2^{p_1} A(h) - A(2h)}{2^{p_1} - 1} = A + \frac{2^{p_2} - 1}{2^{p_1} - 1} h^{p_2} A_2 + \frac{2^{p_3} - 1}{2^{p_1} - 1} h^{p_3} A_3 + \cdots \quad .$$

In other words, the *extrapolated* approximation

$$A^{(1)}(h) = \frac{2^{p_1} A(h) - A(2h)}{2^{p_1} - 1} \tag{16}$$

has order of accuracy $p_2 > p_1$ and asymptotic error expansion

$$A^{(1)}(h) = A + h^{p_2} A_2^{(1)} + h^{p_3} A_3^{(1)} + \cdots \ ,$$

where $A_2^{(1)} = \dfrac{2^{p_2} - 1}{2^{p_1} - 1} A_2$, and so on.

Richardson extrapolation can be repeated to remove more asymptotic error terms. For example,

$$A^{(2)}(h) = \frac{2^{p_2} A^{(1)}(h) - A^{(1)}(2h)}{2^{p_2} - 1}$$

has order p_3. Since $A^{(1)}$ depends on $A(h)$ and $A(2h)$, $A^{(2)}$ depends on $A(h)$, $A(2h)$, and $A(4h)$. It is not necessary to use powers of 2, but this is natural in many applications. Richardson extrapolation *will not work* if the underlying approximation, $A(h)$, has accuracy of order h^p in the $O(h^p)$ sense without at least one term of an asymptotic expansion.

As an example, we derive higher order difference approximations from low order ones. Start, for example, with the first order one sided approximation to $f'(x)$ given by (8a). Taking $p_1 = 1$ in (16) leads to the second order approximation

$$\begin{aligned} f'(x) &\cong 2 \cdot \frac{f(x+h) - f(x)}{h} - \frac{f(x+2h) - f(x)}{2h} \\ &= \frac{-f(x+2h) + 4f(x+h) - 3f(x)}{2h} \ , \end{aligned}$$

which is the second order three point one sided difference approximation (8d). Starting with the second order centered approximation (8c) (with $p_1 = 2$ and $p_2 = 4$) leads to the fourth order approximation (8e).

Richardson extrapolation may also be applied to the output of a complex code. Run it with step size h and $2h$ and apply (16) to the output. This is sometimes applied to stochastic differential equations as an alternative to making up high order schemes from scratch, which can be time consuming and intricate.

When Richardson extrapolation is applied to integration using the trapezoid rule, the resulting integration method is called Romberg integration.

4.2 Convergence analysis

It is important to find ways to test whether a code and the algorithm it is based on are correct. A very useful test, "convergence analysis", is based on the asymptotic error expansion (14). It tests not only whether the error is going to zero as $h \to 0$, but whether it does so as predicted by theory. Suppose, for example, we program the formula (8e) but with 3 instead of 4. The resulting approximation will converge to $f'(x)$ as $h \to 0$ but with the wrong order fo accuracy. A convergence analysis would uncover this immediately.

There are two cases, the case where the exact answer is known and the case where it is not known. While we probably would not write a code for a problem to which we know the answer, it is often possible to apply a code to a problem with a known answer for debugging. In fact, a code should be written modularly so that it is easy to apply it to a range or problems broad enough to include a nontrivial problem[3] with a known answer.

If A is known, we can run the code with step size h and $2h$ and, from the resulting approximations, $A(h)$ and $A(2h)$, compute

$$\begin{aligned} E(h) &\cong A_1 h^{p_1} + A_2 h^{p_2} + \cdots \ , \\ E(2h) &\cong 2^{p_1} A_1 h^{p_1} + 2^{p_2} A_2 h^{p_2} + \cdots \ , \end{aligned}$$

For small h the first term is a good enough approximation so that the ratio should be approximately the characteristic value

$$R(h) = \frac{E(2h)}{E(h)} \cong 2^{p_1}$$

Figure 1 is a computational illustration of this phenomenon. Figure 2 shows what may happen when we apply this convergence analysis to an approximation that is second order accurate in the big O sense without having an asymptotic error expansion. The error gets very small but the error ratio does not have simple behavior as in Figure 1.

Convergence analysis can be applied even when A is not known. In this case we need three approximations, $A(4h)$, $A(2h)$, and $A(h)$. Again assuming the existence of an asymptotic error expansion (8), we get, for small h,

$$R'(h) = \frac{A(4h) - A(2h)}{A(2h) - A(h)} \approx 2^{p_1} \ .$$

5 Integration

Here the Answer we want is the integral

$$I = \int_a^b f(x)dx \ .$$

We discuss only "panel methods" here. Other elegant methods such as Gauss quadrature are discussed in Dahlquist and Bjork and other places. In a panel method, the integration interval, $[a, b]$, is divided into n subintervals, or panels, $P_k = [x_k, x_{k+1}]$, where $a = x_0 < x_1 < \cdots < x_n = b$. If the panel P_k is small, we can get an accurate approximation to

$$I_k = \int_{P_k} f(x)dx = \int_{x_k}^{x_{k+1}} f(x)dx$$

using a few evaluations of f inside P_k. Adding these approximations over k given an approximation to the integral I. Some of the more common panel integral approximations are given in Figure 3. There $x_{k+1/2} = (x_{k+1} + x_k)/2$ is the midpoint of the panel.

[3] A trivial problem is one that is too simple to test the code fully. For example, if you compute the derivative of a linear function, any of the formulae (8a) – (8e) would give the exact answer. There would be no truncation error for the convergence analysis to measure. The fourth order approximation (8e) gives the exact answer for any polynomial of degree less than five.

Rectangle	$I_k \approx hf(x_k)$	1^{st} order
Trapezoid	$I_k \approx \frac{h}{2}\left(f(x_k) + f(x_{k+1})\right)$	2^{nd} order
Midpoint	$I_k \approx hf(x_{k+1/2})$	2^{nd} order
Simpson	$I_k \approx \frac{h}{6}\Big(f(x_k) + 6f(x_{k+1/2}) + f(x_{k+1})\Big)$	4^{th} order
2 point GQ	$I_k \approx \frac{h}{2}\left(f(x_{k+1/2} - \frac{h}{2\sqrt{3}}) + f(x_{k+1/2} + \frac{h}{2\sqrt{3}})\right)$	4^{th} order
3 point GQ	$I_k \approx \frac{h}{18}\left(5f(x_{k+1/2} - \frac{h}{2\sqrt{\frac{3}{5}}}) + 8f(x_{k+1/2}) + 5f(x_{k+1/2} + \frac{h}{2\sqrt{\frac{3}{5}}})\right)$	6^{th} order

Figure 3: Common panel integration rules

We begin our error analysis of panel methods assuming that all the panels are the same size

$$h = \Delta x = |P_k| = x_{k+1} - x_k \text{ for all } k.$$

Given this restriction, not every value of h is allowed. When we take $h \to 0$, we will assume that h only takes allowed values $h = (b-a)/n$ for some integer n.

The overall integration error is the sum of the integration errors for the individual panels. To focus on a particular panel, suppose that P is a generic interval of length h, that is $P = [x_*, x_* + h]$. For the rectangle rule, we approximate

$$I_P = \int_P f(x)dx = \int_{x_*}^{x_*+h} f(x)dx$$

with the approximate integral, $I_P(h)$, defined by

$$I_P(h) = hf(x_*) \quad .$$

To estimate the difference between I_P and $I_P(h)$, we expand f in a Taylor series about x_*:

$$f(x) \approx f(x_*) + (x - x_*)f'(x_*) + \frac{(x-x_*)^2}{2}f''(x_*) + \cdots \quad .$$

Integrating this term by term leads to

$$\begin{aligned} I_P(x_*) &= \int_P f(x_*)dx + \int_P (x - x_*)f'(x_*)dx + \cdots \\ &= hf(x_*) + \frac{h^2}{2}f'(x_*) + \frac{h^3}{6}f''(x_*) + \cdots \quad . \end{aligned}$$

The error in integration over this panel then is

$$E(P,h) = I_P(h) - I_P \approx -\frac{h^2}{2}f'(x_*) - \frac{h^3}{6}f''(x_*) - \cdots \quad . \tag{17}$$

From this we see that the error in integration over any particular panel is on the order of h^2. This leads to a global integration error on the order of h because the number of panels is $n = (b-a)/h$. In other words, the *local truncation error* of order h^2 adds up to lead to a *global error* of order h.

To see this more precisely and construct the asymptotic error expansion, we sum the local for the panels over all panels to get the total error

$$E_{\text{tot}} = \sum_{n=0}^{n-1} E(P_k, h) \approx -\sum_{n=0}^{n-1} \frac{h^2}{2} f'(x_k) - \sum_{n=0}^{n-1} \frac{h^3}{6} f''(x_k) - \cdots \quad . \tag{18}$$

The first term on the right is generally the largest for small h. We can understand it as follows. Since

$$h \sum_{n=0}^{n-1} f(x_k) = \int_a^b f(x)dx + O(h) \quad ,$$

we have

$$h \sum_{n=0}^{n-1} f'(x_k) = \int_a^b f'(x)dx + O(h) = f(b) - f(a) + O(h) \quad .$$

With this approximation, we see that

$$E_{\text{tot}} \approx -\frac{f}{2}\left(f(b) - f(a)\right) + O(h^2) \quad . \tag{19}$$

This gives the first term in the asymptotic error expansion. To get the next term, apply (18) to the error itself, i.e.

$$\begin{aligned} h \sum_{n=0}^{n-1} f'(x_k) &= \int_a^b f'(x)dx - \frac{h}{2}\left(f''(b) - f''(a)\right) + O(h^2) \\ &= f(b) - f(a) - \frac{h}{2}\left(f''(b) - f''(a)\right) + O(h^2) \quad . \end{aligned}$$

In the same way, we find that

$$\frac{h^3}{6} \sum_{n=0}^{n-1} f''(x_k) = \frac{h^2}{6}\left(f'(b) - f'(a)\right) + O(h^3) \quad .$$

Combing all these gives the first two terms in the total error expansion

$$E_{\text{tot}} \approx -\frac{h}{2}\left(f(b) - f(a)\right) + \frac{h^2}{12}\left(f'(b) - f'(a)\right) + \cdots \quad . \tag{20}$$

It is clear that this procedure can be used to continue the expansion as far as we want, but you would have to be very determined to compute, for example, A_4,the coefficient of h^4. An elegant and much more systematic discussion of this error expansion is carried out in the book of Dahlquist and Bjork. The resulting error expansion is called the Euler McLaurin formula. The coefficients $1/2$, $1/12$, and so on, are called Bernoulli numbers.

The error expansion (20) will not be valid if the integrand, f, has singularities inside the domain of integration. Suppose, for example, that $f(x) = 0$ for $x \leq 1/\sqrt{2}$ and $f(x) = \sqrt{x - 1/\sqrt{2}}$ for $x \geq 0$. In this case the error expansion for the rectangle rule approximation

n	Computed Integral	Error	Error/h	$(E - A_1 h)/h^2$	$(E - A_1 h - A_2 h^2)/h^3$
10	3.2271	-0.2546	-1.6973	0.2900	-0.7250
20	3.3528	-0.1289	-1.7191	0.2901	-0.3626
40	3.4168	-0.0649	-1.7300	0.2901	-0.1813
80	3.4492	-0.0325	-1.7354	0.2901	-0.0907
160	3.4654	-0.0163	-1.7381	0.2901	-0.0453

Figure 4: Computational experiment illustrating the asymptotic error expansion for rectangle rule integration

n	Computed Integral	Error	Error/h	$(E - A_1 h)/h^2$
10	7.4398e-02	-3.1277e-02	-3.1277e-01	-4.2173e-01
20	9.1097e-02	-1.4578e-02	-2.9156e-01	-4.1926e-01
40	9.8844e-02	-6.8314e-03	-2.7326e-01	-1.0635e-01
80	1.0241e-01	-3.2605e-03	-2.6084e-01	7.8070e-01
160	1.0393e-01	-1.7446e-03	-2.7914e-01	-1.3670e+00
320	1.0482e-01	-8.5085e-04	-2.7227e-01	-5.3609e-01
640	1.0526e-01	-4.1805e-04	-2.6755e-01	1.9508e+00
1280	1.0546e-01	-2.1442e-04	-2.7446e-01	-4.9470e+00
2560	1.0557e-01	-1.0631e-04	-2.7214e-01	-3.9497e+00
5120	1.0562e-01	-5.2795e-05	-2.7031e-01	1.4700e+00

Figure 5: Computational experiment illustrating the breakdown of the asymptotic expansion.

to $\int_0^1 f(x)dx$ has one valid term only. This is illustrated in Figure 5. The "Error/h" column shows that the first coefficient, A_1, exists. Moreover, A_1 is given by the formula (20). The numbers is the last column do not tend to a limit. This shows that the coefficient A_2 does not exist. The error expansion does not exist beyond the first term.

The analysis of the higher order integration methods listed in Table 1 will be easier if we use a more symmetric basic panel. From now on, the panel of length h will have x_* in the center, rather at the left end, that is

$$P = [x_* - h/2, x_* + h/2] \quad .$$

If we now expand $f(x)$ in a Taylor series about x_* and integrate term by term, we get

$$\int_P f(x)dx = \int_{x=x_*-\frac{h}{2}}^{x_*+\frac{h}{2}} f(x)dx \approx hf(x_*) + \frac{f''(x_*)}{16}h^3 + \frac{f^{(4)}(x_*)}{384}h^5 + \cdots \quad .$$

For the midpoint rule, this leads to a global error expansion in even powers of h, $E \approx A_1h^2 + A_2h^4 + \cdots$, with $A_1 = (f'(b) - f'(a))/16$. Each of the remaining panel methods is symmetric about the center of the panel. This implies that each of them has local truncation error containing only odd powers of h and global error, E_{tot}, containing only even powers of h.

For the remaining methods, we will not compute the coefficients in the error expansion, but only the leading power of h, the order of accuracy. This can be determined by a simple observation: the order of the local truncation error is one more than the degree of the lowest monomial that is not integrated exactly by the panel method. For example, the rectangle rule integrates $f(x) = x^0 \equiv 1$ exactly but gets $f(x) = x^1 \equiv x$ wrong. The order of the lowest monomial not integrated exactly is 1 so the local truncation error is of the order of h^2. The midpoint rule integrates x^0 and x^1 correctly but gets x^2 wrong. The order of the lowest monomial not integrated exactly is 2 so the local truncation error is of the order of h^3. If the generic panel has x_* in the center, then

$$\int_P (x - x_*)^n \, dx$$

is always done exactly if n is odd. This is because both the exact integral and its panel method approximation are zero by symmetry. The exact integral because the panel is symmetric about x_* and the discrete approximation to it because the evaluation points and weights are also symmetric about x_*. This is not true of the rectangle rule.

To understand why this rule works, think of the Taylor expansion of a general function, $f(x)$ about the midpoint, x_*. This is the same as writing f as the sum of a series of monomials. Applying the panel integral approximation to f is the same as applying the approximation to each monomial and summing the results. Moreover, the integral of a monomial $(x - x_*)^n$ over P is proportional to h^{n+1}, as is the panel method approximation to it, regardless of whether the panel method is exact or not. The first monomial that is not integrated exactly contributes something proportional to h^{n+1} to the error.

Using this rule it is easy to determine the accuracy of the approximations in Table 1. The trapezoid rule integrates constants and linear functions exactly, but it gets quadratics wrong. This makes the local truncation error third order and the global error second order. The Simpson's rule coefficients 1/6 and 2/3 are designed exactly to integrate constants and quadratics exactly, which they do. Simpson's rule integrates cubics exactly (by symmetry) but quartics are gotten wrong. This makes Simpson's rule have fourth order global accuracy. The two point Gauss quadrature also does constants and quadratics correctly but quartics wrong (check this!). The three point Gauss quadrature rule does constants, quadratics, and quartics correctly but gets $(x - x_*)^6$ wrong. That makes it sixth order accurate. The theory of Gauss quadrature is discussed by Dahlquist and Bjork. I think it is the most beautiful part of numerical analysis.