CHAPTER 4

Truncation Errors and the Taylor Series

Truncation errors are those that result from using an approximation in place of an exact mathematical procedure. For example, in Chap. 1 we approximated the derivative of velocity of a falling parachutist by a finite-divided-difference equation of the form [Eq. (1.11)]

$$\frac{dv}{dt} \cong \frac{\Delta v}{\Delta t} = \frac{v(t_{i+1}) - v(t_i)}{t_{i+1} - t_i} \tag{4.1}$$

A truncation error was introduced into the numerical solution because the difference equation only approximates the true value of the derivative (recall Fig. 1.4). In order to gain insight into the properties of such errors, we now turn to a mathematical formulation that is used widely in numerical methods to express functions in an approximate fashion—the Taylor series.

4.1 THE TAYLOR SERIES

Taylor's theorem (Box 4.1) and its associated formula, the Taylor series, is of great value in the study of numerical methods. In essence, the *Taylor series* provides a means to predict a function value at one point in terms of the function value and its derivatives at another point. In particular, the theorem states that any smooth function can be approximated as a polynomial.

A useful way to gain insight into the Taylor series is to build it term by term. For example, the first term in the series is

$$f(x_{i+1}) \cong f(x_i) \tag{4.2}$$

This relationship, called the *zero-order approximation,* indicates that the value of f at the new point is the same as its value at the old point. This result makes intuitive sense because if x_i and x_{i+1} are close to each other, it is likely that the new value is probably similar to the old value.

Equation (4.2) provides a perfect estimate if the function being approximated is, in fact, a constant. However, if the function changes at all over the interval, additional terms

Box 4.1 Taylor's Theorem

Taylor's Theorem

If the function f and its first $n + 1$ derivatives are continuous on an interval containing a and x, then the value of the function at x is given by

$$f(x) = f(a) + f'(a)(x-a) + \frac{f''(a)}{2!}(x-a)^2 + \frac{f^{(3)}(a)}{3!}(x-a)^3 + \cdots + \frac{f^{(n)}(a)}{n!}(x-a)^n + R_n \tag{B4.1.1}$$

where the remainder R_n is defined as

$$R_n = \int_a^x \frac{(x-t)^n}{n!} f^{(n+1)}(t)\,dt \tag{B4.1.2}$$

where t = a dummy variable. Equation (B4.1.1) is called the *Taylor series* or *Taylor's formula*. If the remainder is omitted, the right side of Eq. (B4.1.1) is the Taylor polynomial approximation to $f(x)$. In essence, the theorem states that any smooth function can be approximated as a polynomial.

Equation (B4.1.2) is but one way, called the *integral form*, by which the remainder can be expressed. An alternative formulation can be derived on the basis of the integral mean-value theorem.

First Theorem of Mean for Integrals

If the function g is continuous and integrable on an interval containing a and x, then there exists a point ξ between a and x such that

$$\int_a^x g(t)\,dt = g(\xi)(x-a) \tag{B4.1.3}$$

In other words, this theorem states that the integral can be represented by an average value for the function $g(\xi)$ times the interval length $x - a$. Because the average must occur between the minimum and maximum values for the interval, there is a point $x = \xi$ at which the function takes on the average value.

The first theorem is in fact a special case of a second mean-value theorem for integrals.

Second Theorem of Mean for Integrals

If the functions g and h are continuous and integrable on an interval containing a and x, and h does not change sign in the interval, then there exists a point ξ between a and x such that

$$\int_a^x g(t)h(t)\,dt = g(\xi)\int_a^x h(t)\,dt \tag{B4.1.4}$$

Thus, Eq. (B4.1.3) is equivalent to Eq. (B4.1.4) with $h(t) = 1$.

The second theorem can be applied to Eq. (B4.1.2) with

$$g(t) = f^{(n+1)}(t) \qquad h(t) = \frac{(x-t)^n}{n!}$$

As t varies from a to x, $h(t)$ is continuous and does not change sign. Therefore, if $f^{(n+1)}(t)$ is continuous, then the integral mean-value theorem holds and

$$R_n = \frac{f^{(n+1)}(\xi)}{(n+1)!}(x-a)^{n+1}$$

This equation is referred to as the *derivative* or *Lagrange form* of the remainder.

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of the Taylor series are required to provide a better estimate. For example, the *first-order approximation* is developed by adding another term to yield

$$f(x_{i+1}) \cong f(x_i) + f'(x_i)(x_{i+1} - x_i) \tag{4.3}$$

The additional first-order term consists of a slope $f'(x_i)$ multiplied by the distance between x_i and x_{i+1}. Thus, the expression is now in the form of a straight line and is capable of predicting an increase or decrease of the function between x_i and x_{i+1}.

Although Eq. (4.3) can predict a change, it is exact only for a straight-line, or *linear*, trend. Therefore, a *second-order* term is added to the series to capture some of the curvature that the function might exhibit:

$$f(x_{i+1}) \cong f(x_i) + f'(x_i)(x_{i+1} - x_i) + \frac{f''(x_i)}{2!}(x_{i+1} - x_i)^2 \tag{4.4}$$

In a similar manner, additional terms can be included to develop the complete Taylor series expansion:

$$f(x_{i+1}) = f(x_i) + f'(x_i)(x_{i+1} - x_i) + \frac{f''(x_i)}{2!}(x_{i+1} - x_i)^2 + \frac{f^{(3)}(x_i)}{3!}(x_{i+1} - x_i)^3 + \cdots + \frac{f^{(n)}(x_i)}{n!}(x_{i+1} - x_i)^n + R_n \tag{4.5}$$

Note that because Eq. (4.5) is an infinite series, an equal sign replaces the approximate sign that was used in Eqs. (4.2) through (4.4). A remainder term is included to account for all terms from $n + 1$ to infinity:

$$R_n = \frac{f^{(n+1)}(\xi)}{(n+1)!}(x_{i+1} - x_i)^{n+1} \tag{4.6}$$

where the subscript n connotes that this is the remainder for the nth-order approximation and ξ is a value of x that lies somewhere between x_i and x_{i+1}. The introduction of the ξ is so important that we will devote an entire section (Sec. 4.1.1) to its derivation. For the time being, it is sufficient to recognize that there is such a value that provides an exact determination of the error.

It is often convenient to simplify the Taylor series by defining a step size $h = x_{i+1} - x_i$ and expressing Eq. (4.5) as

$$f(x_{i+1}) = f(x_i) + f'(x_i)h + \frac{f''(x_i)}{2!}h^2 + \frac{f^{(3)}(x_i)}{3!}h^3 + \cdots + \frac{f^{(n)}(x_i)}{n!}h^n + R_n \tag{4.7}$$

where the remainder term is now

$$R_n = \frac{f^{(n+1)}(\xi)}{(n+1)!}h^{n+1} \tag{4.8}$$

EXAMPLE 4.1 Taylor Series Approximation of a Polynomial

Problem Statement. Use zero- through fourth-order Taylor series expansions to approximate the function

$$f(x) = -0.1x^4 - 0.15x^3 - 0.5x^2 - 0.25x + 1.2$$

from $x_i = 0$ with $h = 1$. That is, predict the function's value at $x_{i+1} = 1$.

Solution. Because we are dealing with a known function, we can compute values for $f(x)$ between 0 and 1. The results (Fig. 4.1) indicate that the function starts at $f(0) = 1.2$ and then curves downward to $f(1) = 0.2$. Thus, the true value that we are trying to predict is 0.2.

The Taylor series approximation with $n = 0$ is [Eq. (4.2)]

$$f(x_{i+1}) \simeq 1.2$$

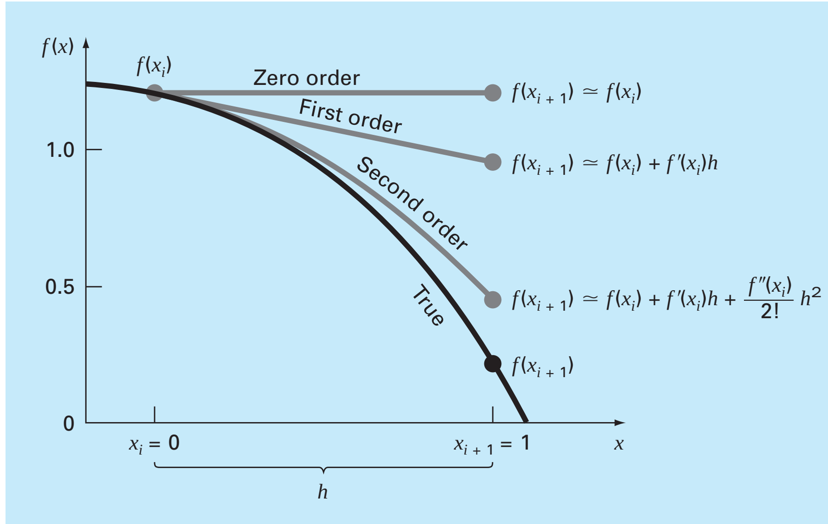

FIGURE 4.1
The approximation of $f(x) = -0.1x^4 - 0.15x^3 - 0.5x^2 - 0.25x + 1.2$ at $x = 1$ by zero-order, first-order, and second-order Taylor series expansions.

Thus, as in Fig. 4.1, the zero-order approximation is a constant. Using this formulation results in a truncation error [recall Eq. (3.2)] of

$$E_t = 0.2 - 1.2 = -1.0$$

at $x = 1$.

For $n = 1$, the first derivative must be determined and evaluated at $x = 0$:

$$f'(0) = -0.4(0.0)^3 - 0.45(0.0)^2 - 1.0(0.0) - 0.25 = -0.25$$

Therefore, the first-order approximation is [Eq. (4.3)]

$$f(x_{i+1}) \simeq 1.2 - 0.25h$$

which can be used to compute $f(1) = 0.95$. Consequently, the approximation begins to capture the downward trajectory of the function in the form of a sloping straight line (Fig. 4.1). This results in a reduction of the truncation error to

$$E_t = 0.2 - 0.95 = -0.75$$

For $n = 2$, the second derivative is evaluated at $x = 0$:

$$f''(0) = -1.2(0.0)^2 - 0.9(0.0) - 1.0 = -1.0$$

Therefore, according to Eq. (4.4),

$$f(x_{i+1}) \simeq 1.2 - 0.25h - 0.5h^2$$

and substituting $h = 1$, $f(1) = 0.45$. The inclusion of the second derivative now adds some downward curvature resulting in an improved estimate, as seen in Fig. 4.1. The truncation error is reduced further to $0.2 - 0.45 = -0.25$.

Additional terms would improve the approximation even more. In fact, the inclusion of the third and the fourth derivatives results in exactly the same equation we started with:

$$f(x) = 1.2 - 0.25h - 0.5h^2 - 0.15h^3 - 0.1h^4$$

where the remainder term is

$$R_4 = \frac{f^{(5)}(\xi)}{5!}h^5 = 0$$

because the fifth derivative of a fourth-order polynomial is zero. Consequently, the Taylor series expansion to the fourth derivative yields an exact estimate at $x_{i+1} = 1$:

$$f(1) = 1.2 - 0.25(1) - 0.5(1)^2 - 0.15(1)^3 - 0.1(1)^4 = 0.2$$

In general, the nth-order Taylor series expansion will be exact for an nth-order polynomial. For other differentiable and continuous functions, such as exponentials and sinusoids, a finite number of terms will not yield an exact estimate. Each additional term will contribute some improvement, however slight, to the approximation. This behavior will be demonstrated in Example 4.2. Only if an infinite number of terms are added will the series yield an exact result.

Although the above is true, the practical value of Taylor series expansions is that, in most cases, the inclusion of only a few terms will result in an approximation that is close enough to the true value for practical purposes. The assessment of how many terms are required to get "close enough" is based on the remainder term of the expansion. Recall that the remainder term is of the general form of Eq. (4.8). This relationship has two major drawbacks. First, ξ is not known exactly but merely lies somewhere between x_i and x_{i+1}. Second, to evaluate Eq. (4.8), we need to determine the $(n+1)$th derivative of $f(x)$. To do this, we need to know $f(x)$. However, if we knew $f(x)$, there would be no need to perform the Taylor series expansion in the present context!

Despite this dilemma, Eq. (4.8) is still useful for gaining insight into truncation errors. This is because we *do* have control over the term h in the equation. In other words, we can choose how far away from x we want to evaluate $f(x)$, and we can control the number of terms we include in the expansion. Consequently, Eq. (4.8) is usually expressed as

$$R_n = O(h^{n+1})$$

where the nomenclature $O(h^{n+1})$ means that the truncation error is of the order of h^{n+1}. That is, the error is proportional to the step size h raised to the $(n+1)$th power. Although this approximation implies nothing regarding the magnitude of the derivatives that multiply h^{n+1}, it is extremely useful in judging the comparative error of numerical methods based on Taylor series expansions. For example, if the error is $O(h)$, halving the step size will halve the error. On the other hand, if the error is $O(h^2)$, halving the step size will quarter the error.

In general, we can usually assume that the truncation error is decreased by the addition of terms to the Taylor series. In many cases, if h is sufficiently small, the first- and other lower-order terms usually account for a disproportionately high percent of the error. Thus, only a few terms are required to obtain an adequate estimate. This property is illustrated by the following example.

EXAMPLE 4.2 Use of Taylor Series Expansion to Approximate a Function with an Infinite Number of Derivatives

Problem Statement. Use Taylor series expansions with $n = 0$ to 6 to approximate $f(x) = \cos x$ at $x_{i+1} = \pi/3$ on the basis of the value of $f(x)$ and its derivatives at $x_i = \pi/4$. Note that this means that $h = \pi/3 - \pi/4 = \pi/12$.

Solution. As with Example 4.1, our knowledge of the true function means that we can determine the correct value $f(\pi/3) = 0.5$.

The zero-order approximation is [Eq. (4.3)]

$$f\left(\frac{\pi}{3}\right) \cong \cos\left(\frac{\pi}{4}\right) = 0.707106781$$

which represents a percent relative error of

$$\varepsilon_t = \frac{0.5 - 0.707106781}{0.5} 100\% = -41.4\%$$

For the first-order approximation, we add the first derivative term where $f'(x) = -\sin x$:

$$f\left(\frac{\pi}{3}\right) \cong \cos\left(\frac{\pi}{4}\right) - \sin\left(\frac{\pi}{4}\right)\left(\frac{\pi}{12}\right) = 0.521986659$$

which has $\varepsilon_t = -4.40$ percent.

For the second-order approximation, we add the second derivative term where $f''(x) = -\cos x$:

$$f\left(\frac{\pi}{3}\right) \cong \cos\left(\frac{\pi}{4}\right) - \sin\left(\frac{\pi}{4}\right)\left(\frac{\pi}{12}\right) - \frac{\cos(\pi/4)}{2}\left(\frac{\pi}{12}\right)^2 = 0.497754491$$

with $\varepsilon_t = 0.449$ percent. Thus, the inclusion of additional terms results in an improved estimate.

The process can be continued and the results listed, as in Table 4.1. Notice that the derivatives never go to zero as was the case with the polynomial in Example 4.1. Therefore, each additional term results in some improvement in the estimate. However, also notice how most of the improvement comes with the initial terms. For this case, by the time we

TABLE 4.1 Taylor series approximation of $f(x) = \cos x$ at $x_{i+1} = \pi/3$ using a base point of $\pi/4$. Values are shown for various orders (n) of approximation.

Order n	$f^{(n)}(x)$	$f(\pi/3)$	ε_t
0	$\cos x$	0.707106781	−41.4
1	$-\sin x$	0.521986659	−4.4
2	$-\cos x$	0.497754491	0.449
3	$\sin x$	0.499869147	2.62×10^{-2}
4	$\cos x$	0.500007551	-1.51×10^{-3}
5	$-\sin x$	0.500000304	-6.08×10^{-5}
6	$-\cos x$	0.499999988	2.44×10^{-6}

have added the third-order term, the error is reduced to 2.62×10^{-2} percent, which means that we have attained 99.9738 percent of the true value. Consequently, although the addition of more terms will reduce the error further, the improvement becomes negligible.

4.1.1 The Remainder for the Taylor Series Expansion

Before demonstrating how the Taylor series is actually used to estimate numerical errors, we must explain why we included the argument ξ in Eq. (4.8). A mathematical derivation is presented in Box 4.1. We will now develop an alternative exposition based on a somewhat more visual interpretation. Then we can extend this specific case to the more general formulation.

Suppose that we truncated the Taylor series expansion [Eq. (4.7)] after the zero-order term to yield

$$f(x_{i+1}) \cong f(x_i)$$

A visual depiction of this zero-order prediction is shown in Fig. 4.2. The remainder, or error, of this prediction, which is also shown in the illustration, consists of the infinite series of terms that were truncated:

$$R_0 = f'(x_i)h + \frac{f''(x_i)}{2!}h^2 + \frac{f^{(3)}(x_i)}{3!}h^3 + \cdots$$

It is obviously inconvenient to deal with the remainder in this infinite series format. One simplification might be to truncate the remainder itself, as in

$$R_0 \cong f'(x_i)h \tag{4.9}$$

FIGURE 4.2
Graphical depiction of a zero-order Taylor series prediction and remainder.