We now turn our attention to the use of numerical methods for solving problems from calculus and differential equations. In this chapter, we investigate numerical techniques for finding derivatives and definite integrals. Several formulas for approximating a first or second derivative by a difference quotient are given. These formulas can be found with the use of Taylor polynomials or Lagrange interpolation polynomials.

Numerical methods approximate the definite integral of a given function by a weighted sum of function values at specified points. We first consider several methods, known as Newton–Cotes formulas, that use evenly spaced data points. These methods are based on the integral of a simple interpolating polynomial. The trapezoid rule uses the function values at the ends of the interval of integration; Simpson’s rule is based on a parabola through the ends of the interval and the midpoint of the interval. Improved accuracy can be obtained by subdividing the interval of integration and applying one of these simple techniques on each subinterval. Finally, we present a powerful integration technique, Gaussian quadrature, in which the points used in evaluating a function are chosen to provide the best possible result for a certain class of functions.

Applications of numerical differentiation are especially common in converting differential equations into difference equations for numerical solution. One must be very careful when using numerical techniques to estimate the rate of change of measured data, since small errors are exaggerated by differentiation. Integration, on the other hand, tends to smooth out errors. Numerical integration is widely used in applications, because some simple functions are difficult or impossible to integrate exactly. We present a few representative problems and use them, together with other examples, to illustrate the techniques of the chapter. We consider techniques for ordinary differential equations in Chapters 12–14 and for partial differential equations in Chapter 15.
Numerical differentiation requires us to find estimates for the derivative or slope of a function by using the function values at only a set of discrete points. We begin by considering methods of approximating a first derivative. We then present formulas for second and higher derivatives. The final topic in our treatment of numerical differentiation is the use of acceleration (introduced in Chapter 1) to improve an approximate derivative value.

11.1.1 First Derivatives

The simplest difference formulas are based on using a straight line to interpolate the given data; that is, they use two data points to estimate the derivative. We assume that we have function values at \( x_{i-1} \), \( x_i \), and \( x_{i+1} \); we let \( f(x_{i-1}) = y_{i-1} \), \( f(x_i) = y_i \), and \( f(x_{i+1}) = y_{i+1} \). The spacing between the values of \( x \) is constant, so that \( h = x_{i+1} - x_i = x_i - x_{i-1} \). Then we have the standard two-point formulas:

**Forward difference formula**

\[
f'(x_i) \approx \frac{f(x_{i+1}) - f(x_i)}{x_{i+1} - x_i} = \frac{y_{i+1} - y_i}{x_{i+1} - x_i}.
\]

**Backward difference formula**

\[
f'(x_i) \approx \frac{f(x_i) - f(x_{i-1})}{x_i - x_{i-1}} = \frac{y_i - y_{i-1}}{x_i - x_{i-1}}.
\]

A more balanced approach gives an approximation to the derivative at \( x_i \) using function values \( f(x_{i-1}) \) and \( f(x_{i+1}) \). Taking the average of the approximations from the forward and backward difference formulas gives the central difference formula.

**Central difference formula**

\[
f'(x_i) \approx \frac{f(x_{i+1}) - f(x_{i-1})}{x_{i+1} - x_{i-1}} = \frac{y_{i+1} - y_{i-1}}{x_{i+1} - x_{i-1}}.
\]

The three kinds of difference formula are shown in Fig. 11.4.

![FIGURE 11.4 Three difference approximations to \( f'(x_i) \).](image)
Example 11.1 Forward, Backward, and Central Differences

To illustrate the three kinds of difference formula, consider the data points \((x_0, y_0) = (1, 2), (x_1, y_1) = (2, 4), (x_2, y_2) = (3, 8), (x_3, y_3) = (4, 16), \) and \((x_4, y_4) = (5, 32)\). Using the forward difference formula, we estimate \(f'(x_2) = f'(3)\), with \(h = 1\), as

\[
f'(x_2) \approx \frac{f(x_3) - f(x_2)}{x_3 - x_2} = \frac{y_3 - y_2}{1} = 16 - 8 = 8.
\]

Using the backward difference formula, we find that

\[
f'(x_2) \approx \frac{f(x_2) - f(x_1)}{x_2 - x_1} = \frac{y_2 - y_1}{1} = 8 - 4 = 4.
\]

With the central difference formula, the estimate for \(f'(x_2)\), with \(h = 1\), is

\[
f'(x_2) \approx \frac{f(x_3) - f(x_1)}{x_3 - x_1} = \frac{y_3 - y_1}{2} = \frac{16 - 4}{2} = 6.
\]

We also observe that we can use any of these formulas with the given data and \(h = 2\). For example, the central difference formula estimate for \(f'(x_2)\) with \(h = 2\) is

\[
f'(x_2) \approx \frac{f(x_4) - f(x_0)}{x_4 - x_0} = \frac{y_4 - y_0}{4} = \frac{32 - 2}{4} = 7.5.
\]

Although it may seem surprising that we would want to use a larger step size (like \(h = 2\)), we will use this result in Example 11.4.

The data are taken from the function \(y = f(x) = 2^x\), so we can compare estimates of the derivative with the true value, found by evaluating \(f'(x) = 2^x \ln(2)\) at \(x = 3\). The result is \(f'(3) \approx 2^3 \ln(2) = 5.544\).

Interpolating the data by a polynomial rather than a straight line gives a difference formula that makes use of more than two data points. The forward and backward three-point formulas are given next.

**Three-point forward difference formula**

\[
f'(x_i) \approx \frac{-f(x_{i+2}) + 4f(x_{i+1}) - 3f(x_i)}{x_{i+2} - x_i} = \frac{-y_{i+2} + 4y_{i+1} - 3y_i}{x_{i+2} - x_i}.
\]

**Three-point backward difference formula**

\[
f'(x_i) \approx \frac{3f(x_i) - 4f(x_{i-1}) + f(x_{i-2})}{x_i - x_{i-2}} = \frac{3y_i - 4y_{i-1} + y_{i-2}}{x_i - x_{i-2}}.
\]

Example 11.2 Three-Point Difference Formulas

We illustrate these difference formulas by using the data from Example 11.1. Using the three point forward difference formula, we find that

\[
f'(x_2) \approx \frac{-y_4 + 4y_3 - 3y_2}{2} = \frac{-32 + 4(16) - 3(8)}{2} = 4.
\]

Using the three-point backward difference formula, we find that

\[
f'(x_2) \approx \frac{3y_2 - 4y_1 + y_0}{2} = \frac{3(8) - 4(4) + 2}{2} = 5.
\]
Discussion

The forward difference formula can be found from the Taylor polynomial with remainder:

$$f(x + h) = f(x) + hf'(x) + \frac{h^2}{2} f''(\eta). \quad (11.1)$$

For \( h = x_{i+1} - x_i \), this gives

$$f'(x_i) = \frac{f(x_{i+1}) - f(x_i)}{h} - \frac{h}{2} f''(\eta),$$

for some \( x_i \leq \eta \leq x_{i+1} \). Thus, the truncation error for the forward difference formula is \( O(h) \). The formula can also be obtained by considering the Lagrange interpolating polynomial for the points \((x_i, y_i)\) and \((x_{i+1}, y_{i+1})\).

Similarly, the backward difference formula can be found from eq. (11.1) by letting \( h = x_{i-1} - x_i \). This gives \( f(x_{i-1}) = f(x_i) + hf'(x_i) + \frac{h^2}{2} f''(\eta), \) or

$$f'(x_i) = \frac{f(x_{i-1}) - f(x_i)}{h} - \frac{h}{2} f''(\eta), \quad \text{for some } x_{i-1} \leq \eta \leq x_i.$$

The central difference formula for the first derivative of \( f \) at the point \( x_i \) can be found from the next higher order Taylor polynomial, with \( h = x_{i+1} - x_i = x_i - x_{i-1} \):

$$f(x_{i+1}) = f(x_i + h) = f(x_i) + hf'(x_i) + \frac{h^2}{2!} f''(x_i) + \frac{h^3}{3!} f'''(\eta_1),$$

$$f(x_{i-1}) = f(x_i - h) = f(x_i) - hf'(x_i) + \frac{h^2}{2!} f''(x_i) - \frac{h^3}{3!} f'''(\eta_2),$$

where \( x \leq \eta_1 \leq x + h \) and \( x - h \leq \eta_2 \leq x \). Although the error term involves the third derivative at two unknown points in two different intervals, if we assume that the third derivative is continuous on \([x - h, x + h] \), we can write the central difference formula with the error term as

$$f'(x_i) = \frac{f(x_{i+1}) - f(x_{i-1})}{2h} + \frac{h^2}{6} f'''(\eta), \quad \text{for some point } x_{i-1} \leq \eta \leq x_{i+1}.$$

The central difference formula can also be found from the three-point Lagrange interpolating polynomial and is therefore known as a three-point formula (although \( f(x_i) \) does not appear in it).

General Three-Point Formulas

Three-point approximation formulas for the first derivative, based on the Lagrange interpolation polynomial, do not require that the data points be equally spaced; given the three points, \((x_1, y_1), (x_2, y_2), \) and \((x_3, y_3)\), with \( x_1 < x_2 < x_3 \), the formula that follows can be used to approximate the derivative at any point in the interval \([x_1, x_3]\). The first derivative at each of the data points is given by
\[ f'(x_1) \approx \frac{2x_1 - x_2 - x_3}{(x_1 - x_2)(x_1 - x_3)} y_1 + \frac{x_1 - x_3}{(x_2 - x_1)(x_2 - x_3)} y_2 \\
+ \frac{x_1 - x_2}{(x_3 - x_1)(x_3 - x_2)} y_3, \]

\[ f'(x_2) \approx \frac{x_2 - x_3}{(x_1 - x_2)(x_1 - x_3)} y_1 + \frac{2x_2 - x_1 - x_3}{(x_2 - x_1)(x_2 - x_3)} y_2 \\
+ \frac{x_2 - x_1}{(x_3 - x_1)(x_3 - x_2)} y_3, \]

\[ f'(x_3) \approx \frac{x_3 - x_2}{(x_1 - x_2)(x_1 - x_3)} y_1 + \frac{x_3 - x_1}{(x_2 - x_1)(x_2 - x_3)} y_2 \\
+ \frac{2x_3 - x_1 - x_2}{(x_3 - x_1)(x_3 - x_2)} y_3. \]

For evenly spaced data, the formula for \( f'(x_2) \) reduces to the central difference formula presented earlier.

As discussed in Chapter 8, the Lagrange interpolation polynomial for the points \((x_1, y_1), (x_2, y_2),\) and \((x_3, y_3)\) can be written as

\[ L(x) = L_1(x)y_1 + L_2(x)y_2 + L_3(x)y_3, \]

where

\[ L_1(x) = \frac{(x - x_2)(x - x_3)}{(x_1 - x_2)(x_1 - x_3)}, \quad L_2(x) = \frac{(x - x_1)(x - x_3)}{(x_2 - x_1)(x_2 - x_3)}, \]

\[ L_3(x) = \frac{(x - x_1)(x - x_2)}{(x_3 - x_1)(x_3 - x_2)}. \]

The approximation to the first derivative of \( f \) comes from \( f'(x) \approx L'(x) \), which can be written as

\[ L'(x) = L'_1(x)y_1 + L'_2(x)y_2 + L'_3(x)y_3, \]

where

\[ L'_1(x) = \frac{2x - x_2 - x_3}{(x_1 - x_2)(x_1 - x_3)}, \quad L'_2(x) = \frac{2x - x_1 - x_3}{(x_2 - x_1)(x_2 - x_3)}, \]

\[ L'_3(x) = \frac{2x - x_1 - x_2}{(x_3 - x_1)(x_3 - x_2)}. \]

Thus,

\[ f'(x) \approx \frac{2x - x_2 - x_3}{(x_1 - x_2)(x_1 - x_3)} y_1 + \frac{2x - x_1 - x_3}{(x_2 - x_1)(x_2 - x_3)} y_2 \\
+ \frac{2x - x_1 - x_2}{(x_3 - x_1)(x_3 - x_2)} y_3. \]
11.1.2 Higher Derivatives

Formulas for higher derivatives can be found by differentiating the interpolating polynomial repeatedly or by using Taylor expansions. For example, given data at three equally spaced abscissas \(x_{i-1}, x_i, \) and \(x_{i+1},\) the formula for the second derivative is

\[
f''(x_i) \approx \frac{1}{h^2} \left[ f(x_{i+1}) - 2f(x_i) + f(x_{i-1}) \right], \quad \text{with truncation error } O(h^2).
\]

**Example 11.3 Second Derivative**

Using the data given in Example 11.1, we estimate the second derivative at \(x_2 = 3,\) using the points \((x_1, y_1) = (2, 4), \) \((x_2, y_2) = (3, 8),\) and \((x_3, y_3) = (4, 16); \) for this example, \(h = 1,\) so we have

\[
f''(3) \approx \left[ f(4) - 2f(3) + f(2) \right] = [16 - 2(8) + 4] = 4.
\]

**Derivation of Second-Derivative Formula**

From the Taylor polynomial with remainder, we find that

\[
f(x + h) = f(x) + hf'(x) + \frac{h^2}{2!} f''(x) + \frac{h^3}{3!} f'''(x) + \frac{h^4}{4!} f^{(4)}(\eta_1),
\]

\[
f(x - h) = f(x) - hf'(x) + \frac{h^2}{2!} f''(x) - \frac{h^3}{3!} f'''(x) + \frac{h^4}{4!} f^{(4)}(\eta_2),
\]

where \(x \leq \eta_1 \leq x + h\) and \(x - h \leq \eta_2 \leq x.\) Adding gives

\[
f(x + h) + f(x - h) = 2f(x) + h^2 f''(x) + \frac{h^4}{4!} \left[ f^{(4)}(\eta_1) + f^{(4)}(\eta_2) \right],
\]

or \(f''(x) \approx \frac{1}{h^2} \left[ f(x + h) - 2f(x) + f(x - h) \right],\) with truncation error \(O(h^4).\) The error depends on even powers of \(h.\) If we assume that the fourth derivative is continuous on \([x - h, x + h],\) we can write the error term as \(-\frac{h^4}{12} f^{(4)}(\eta)\) for some point \(x - h \leq \eta \leq x + h.\)

To find formulas for the third and fourth derivatives, we seek a linear combination of the Taylor expansions for \(f(x + 2h), f(x + h), f(x - h),\) and \(f(x - 2h)\) so that all derivatives below the desired derivative cancel. Table 11.1 gives these formulas.

**Table 11.1** Centered difference formulas, all \(O(h^2).\)

\[
f'(x_i) \approx \frac{1}{2h} \left[ f(x_{i+1}) - f(x_{i-1}) \right]
\]

\[
f''(x_i) \approx \frac{1}{h^2} \left[ f(x_{i+1}) - 2f(x_i) + f(x_{i-1}) \right]
\]

\[
f'''(x_i) \approx \frac{1}{2h^3} \left[ f(x_{i+2}) - 2f(x_{i+1}) + 2f(x_{i-1}) - f(x_{i-2}) \right]
\]

\[
f''''(x_i) \approx \frac{1}{h^4} \left[ f(x_{i+2}) - 4f(x_{i+1}) + 6f(x_i) - 4f(x_{i-1}) + f(x_{i-2}) \right]
\]
Partial Derivatives

Finite-difference approximations for partial derivatives of a function of two variables are based on a discrete mesh of points for both variables. We denote a general point as \((x, y)\) and the value of the function \(u(x, y)\) at that point as \(u_{ij}\); the spacing in the \(x\) and \(y\) directions is the same, \(h\). The simplest partial-derivative formulas are direct analogs of the preceding ordinary-derivative formulas; we use subscripts to indicate partial differentiation. Also, each formula is given in a schematic form, indicating only the coefficients on each function value. All of the following formulas are \(O(h^3)\); the approximation to each partial derivative is given at \((x, y)\):

\[
u_x \approx \frac{1}{2h} [-u_{i-1,j} + u_{i+1,j}] \approx \frac{1}{2h} \begin{bmatrix} -1 & 0 & 1 \end{bmatrix} j; \]

\[
u_{xx} \approx \frac{1}{h^2} [u_{i-1,j} - 2u_{i,j} + u_{i+1,j}] \approx \frac{1}{h^2} \begin{bmatrix} 1 & -2 & 1 \end{bmatrix} j.\]

For the mixed second partial derivative and higher derivatives, the schematic form is especially convenient. The Laplacian operator is \(\nabla^2 u = u_{xx} + u_{yy}\), and the biharmonic operator is \(\nabla^4 u = u_{xxxx} + 2u_{xxyy} + u_{yyyy}\). We thus have:

\[
u_{xy} \approx \frac{1}{4h^2} \begin{bmatrix} -1 & 0 & 1 \end{bmatrix} j+1 \]

\[
\nabla^2 u \approx \frac{1}{h^2} \begin{bmatrix} 1 & -4 & 1 \end{bmatrix} j+1 \]

\[
\nabla^4 u \approx \frac{1}{h^4} \begin{bmatrix} 1 & 2 & 2 & 1 \end{bmatrix} j+1 \]

(See Ames, 1992, for a discussion of these and other formulas.)
(a) Forward difference representations

<table>
<thead>
<tr>
<th></th>
<th>$f_j$</th>
<th>$f_{j+1}$</th>
<th>$f_{j+2}$</th>
<th>$f_{j+3}$</th>
<th>$f_{j+4}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$hf'(x_j)$</td>
<td>-1</td>
<td>1</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>$(h^2)f''(x_j)$</td>
<td>1</td>
<td>-2</td>
<td>1</td>
<td></td>
<td></td>
</tr>
<tr>
<td>$(h^3)f'''(x_j)$</td>
<td>-1</td>
<td>3</td>
<td>-3</td>
<td>1</td>
<td></td>
</tr>
<tr>
<td>$(h^4)f''''(x_j)$</td>
<td>1</td>
<td>-4</td>
<td>6</td>
<td>-4</td>
<td>1</td>
</tr>
</tbody>
</table>

$+ O(h)$

(b) Backward difference representations

<table>
<thead>
<tr>
<th></th>
<th>$f_{j-4}$</th>
<th>$f_{j-3}$</th>
<th>$f_{j-2}$</th>
<th>$f_{j-1}$</th>
<th>$f_j$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$hf'(x_j)$</td>
<td></td>
<td>-1</td>
<td></td>
<td>1</td>
<td></td>
</tr>
<tr>
<td>$(h^2)f''(x_j)$</td>
<td></td>
<td></td>
<td>1</td>
<td>-2</td>
<td>1</td>
</tr>
<tr>
<td>$(h^3)f'''(x_j)$</td>
<td></td>
<td>-1</td>
<td>3</td>
<td>-3</td>
<td>1</td>
</tr>
<tr>
<td>$(h^4)f''''(x_j)$</td>
<td></td>
<td>1</td>
<td>-4</td>
<td>6</td>
<td>-4</td>
</tr>
</tbody>
</table>

$+ O(h)$

Fig. 3.2 Forward and backward difference representations of $O(h)$.

(a) Forward difference representations

<table>
<thead>
<tr>
<th></th>
<th>$f_i$</th>
<th>$f_{i+1}$</th>
<th>$f_{i+2}$</th>
<th>$f_{i+3}$</th>
<th>$f_{i+4}$</th>
<th>$f_{i+5}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$hf'(x_i)$</td>
<td>-3</td>
<td>4</td>
<td>-1</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>$(h^2)f''(x_i)$</td>
<td>2</td>
<td>-5</td>
<td>4</td>
<td>-1</td>
<td></td>
<td></td>
</tr>
<tr>
<td>$(h^3)f'''(x_i)$</td>
<td>-5</td>
<td>18</td>
<td>-24</td>
<td>14</td>
<td>-3</td>
<td></td>
</tr>
<tr>
<td>$(h^4)f''''(x_i)$</td>
<td>3</td>
<td>-14</td>
<td>26</td>
<td>-24</td>
<td>11</td>
<td>-2</td>
</tr>
</tbody>
</table>

$O(h)^2$

(b) Backward difference representations

<table>
<thead>
<tr>
<th></th>
<th>$f_{i-5}$</th>
<th>$f_{i-4}$</th>
<th>$f_{i-3}$</th>
<th>$f_{i-2}$</th>
<th>$f_{i-1}$</th>
<th>$f_i$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$hf'(x_i)$</td>
<td></td>
<td></td>
<td>1</td>
<td>-4</td>
<td>3</td>
<td></td>
</tr>
<tr>
<td>$(h^2)f''(x_i)$</td>
<td></td>
<td></td>
<td>-1</td>
<td>4</td>
<td>-5</td>
<td>2</td>
</tr>
<tr>
<td>$(h^3)f'''(x_i)$</td>
<td></td>
<td>3</td>
<td>-14</td>
<td>24</td>
<td>-18</td>
<td>5</td>
</tr>
<tr>
<td>$(h^4)f''''(x_i)$</td>
<td></td>
<td>-2</td>
<td>11</td>
<td>-24</td>
<td>26</td>
<td>-14</td>
</tr>
</tbody>
</table>

$O(h)^2$

Fig. 3.3 Forward and backward difference representations of $O(h)^2$. 
(a) Representations of $O(h)^2$

<table>
<thead>
<tr>
<th></th>
<th>$f_{j-2}$</th>
<th>$f_{j-1}$</th>
<th>$f_j$</th>
<th>$f_{j+1}$</th>
<th>$f_{j+2}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$2hf'(x_j)$=</td>
<td></td>
<td>-1</td>
<td>0</td>
<td>1</td>
<td></td>
</tr>
<tr>
<td>$(h^2)f''(x_j)$=</td>
<td>1</td>
<td>-2</td>
<td>1</td>
<td></td>
<td></td>
</tr>
<tr>
<td>$2(h^3)f'''(x_j)$=</td>
<td>-1</td>
<td>2</td>
<td>0</td>
<td>-2</td>
<td>1</td>
</tr>
<tr>
<td>$(h^4)f''''(x_j)$=</td>
<td>1</td>
<td>-4</td>
<td>6</td>
<td>-4</td>
<td>1</td>
</tr>
</tbody>
</table>

(b) Representations of $O(h)^4$

<table>
<thead>
<tr>
<th></th>
<th>$f_{j-3}$</th>
<th>$f_{j-2}$</th>
<th>$f_{j-1}$</th>
<th>$f_j$</th>
<th>$f_{j+1}$</th>
<th>$f_{j+2}$</th>
<th>$f_{j+3}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$12hf'(x_j)$=</td>
<td></td>
<td>1</td>
<td>-8</td>
<td>0</td>
<td>8</td>
<td>-1</td>
<td></td>
</tr>
<tr>
<td>$12(h^2)f''(x_j)$=</td>
<td>-1</td>
<td>16</td>
<td>-30</td>
<td>16</td>
<td>-1</td>
<td></td>
<td></td>
</tr>
<tr>
<td>$8(h^3)f'''(x_j)$=</td>
<td>1</td>
<td>-8</td>
<td>13</td>
<td>0</td>
<td>-13</td>
<td>8</td>
<td>-1</td>
</tr>
<tr>
<td>$6(h^4)f''''(x_j)$=</td>
<td>-1</td>
<td>12</td>
<td>-39</td>
<td>56</td>
<td>-39</td>
<td>12</td>
<td>-1</td>
</tr>
</tbody>
</table>

Fig. 3.4 Central difference representations.
11.1.3 Richardson Extrapolation

The technique known as Richardson extrapolation, introduced in Chapter 1, provides a method of improving the accuracy of a low-order approximation formula $A(h)$ whose error can be expressed as

$$A - A(h) = a_2 h^2 + a_4 h^4 + \ldots,$$

where $A$ is the true (unknown) value of the quantity being approximated by $A(h)$ and the coefficients of the error terms do not depend on the step size $h$. To apply Richardson extrapolation, we form approximations to $A$ separately using the step sizes $h$ and $h/2$. These are combined to give an $O(h^2)$ approximation to $A$ by means of two applications of an $O(h^2)$ formula:

$$A = \frac{4A(h/2) - A(h)}{3}.$$

To continue the extrapolation process, consider

$$A = B(h) + b_4 h^4 + b_6 h^6 + b_8 h^8 + \ldots,$$

where $B(h)$ is simply the extrapolated approximation to $A$, using step sizes $h$ and $h/2$. If we can also find an approximation to $A$ using step sizes $h/2$ and $h/4$, this would correspond to $B(h/2)$. If we extrapolate using $B(h)$ and $B(h/2)$, we get

$$C(h) \approx \frac{16B(h/2) - B(h)}{15},$$

which has error $O(h^6)$.

The central difference formula can be written as

$$D(h) = f'(x) = \frac{1}{2h} [f(x + h) - f(x - h)] - \frac{h^2}{6} f'''(x) + O(h^4).$$

We can also find $f'(x)$ using one-half the previous value of $h$ (whatever it may have been):

$$D(h/2) = f'(x) = \frac{1}{h} [f(x + h/2) - f(x - h/2)] - \frac{h^2}{24} f'''(x) + O(h^4).$$

Since the coefficient of the $h^2$ term does not change (although we do not, in general, know its value), the two estimates can be combined to give

$$D = \frac{4D(h/2) - D(h)}{3}.$$
Example 11.4 Improved Estimate of the Derivative

We illustrate the use of Richardson extrapolation with the values from Example 11.1. The value of \( h \) is 2, and the approximation to \( f'(x) \) is based on \( D(h) = 7.5 \) and \( D(h/2) \). We have

\[
D = \frac{4(6) - 7.5}{3} = \frac{16.5}{3} \approx 5.5.
\]

The data in the example are points on the curve \( f(x) = 2^x \). The actual value of \( f'(x) \) is \((\ln 2)2^x\), which gives \( f'(3) \approx 5.54\).

Discussion

Richardson extrapolation forms a linear combination of approximations \( A(h) \) and \( A(h/2) \), the first using a step size \( h \), the second based on half the original step size; the combination is chosen so that the dominant error term, which depends on \( h^2 \), cancels. Representing \( A \) in terms of the approximation and the error terms, we have

\[
A = A(h) + a_2 h^2 + a_4 h^4 + \ldots
\]  

(11.2)

If the same approximation formula is used with step size \( h/2 \) in place of \( h \), the true value can be expressed as

\[
A = A(h/2) + a_2 \frac{h^2}{4} + a_4 \frac{h^4}{16} + \ldots,
\]

or

\[
4A = 4A(h/2) + a_2 h^2 + a_4 \frac{h^4}{4} + \ldots
\]  

(11.3)

Subtracting eq. (11.2) from eq. (11.3) gives

\[
3A = 4A(h/2) - A(h) + O(h^4),
\]

or

\[
A = \frac{1}{3} [4A(h/2) - A(h)] + O(h^4).
\]

The \( h^2 \) error terms cancel, although the higher order terms do not. However, we now have an \( O(h^4) \) approximation to \( A \) derived by using two applications of an \( O(h^2) \) formula.
To continue the extrapolation, we write

\[ A = B(h) + b_4 h^4 + b_6 h^6 + b_8 h^8 + \ldots, \]  

(11.4)

where \( B(h) \) is simply the extrapolated approximation to \( A \), using step sizes \( h \) and \( h/2 \). If we can also find an approximation to \( A \) using step sizes \( h/2 \) and \( h/4 \), this would correspond to \( B(h/2) \). We begin with \( B(h/2) \)

\[ A = B(h/2) + b_4 (h^4/16) + b_6 (h^6/64) + b_8 (h^8/256) + \ldots. \]  

(11.5)

Multiplying eq. (11.5) by 16 and subtracting eq. (11.4) from the result, so that the \( h^4 \) terms cancel, yields

\[ 15A = 16B(h/2) - B(h) + c_6 h^6 + c_8 h^8 + \ldots. \]

Now we define the second-level extrapolated approximation to \( A \) as

\[ C(h) \approx (16B(h/2) - B(h))/15. \]