MAP 2220 – FUNDAMENTOS DE ANÁLISE NUMÉRICA

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4 Numerical Differentiation and Integration 173

4.1 Numerical Differentiation 174
4.2 Richardson's Extrapolation 185
4.3 Elements of Numerical Integration 193
4.4 Composite Numerical Integration 203
4.5 Romberg Integration 213
4.6 Adaptive Quadrature Methods 220
4.7 Gaussian Quadrature 228
4.8 Multiple Integrals 235
4.9 Improper Integrals 250
4.10 Survey of Methods and Software 256

4.1 Numerical Differentiation

The derivative of the function f at x_0 is

$$f'(x_0) = \lim_{h\to 0} \frac{f(x_0+h) - f(x_0)}{h}.$$

This formula gives an obvious way to generate an approximation to $f'(x_0)$; simply compute

$$\frac{f(x_0+h) - f(x_0)}{h}$$

for small values of h. Although this may be obvious, it is not very successful, due to our old nemesis round-off error. But it is certainly a place to start.

To approximate $f'(x_0)$, suppose first that $x_0 \in (a, b)$, where $f \in C^2[a, b]$, and that $x_1 = x_0 + h$ for some $h \neq 0$ that is sufficiently small to ensure that $x_1 \in [a, b]$. We construct the first Lagrange polynomial $P_{0,1}(x)$ for f determined by x_0 and x_1, with its error term:

$$\begin{aligned} f(x) &= P_{0,1}(x) + \frac{(x-x_0)(x-x_1)}{2!} f''(\xi(x)) \\ &= \frac{f(x_0)(x-x_0-h)}{-h} + \frac{f(x_0+h)(x-x_0)}{h} + \frac{(x-x_0)(x-x_0-h)}{2} f''(\xi(x)), \end{aligned}$$

for some $\xi(x)$ between x_0 and x_1. Differentiating gives

$$\begin{aligned} f'(x) &= \frac{f(x_0+h) - f(x_0)}{h} + D_x\left[\frac{(x-x_0)(x-x_0-h)}{2} f''(\xi(x))\right] \\ &= \frac{f(x_0+h) - f(x_0)}{h} + \frac{2(x-x_0) - h}{2} f''(\xi(x)) \\ &\quad + \frac{(x-x_0)(x-x_0-h)}{2} D_x(f''(\xi(x))). \end{aligned}$$

Deleting the terms involving $\xi(x)$ gives

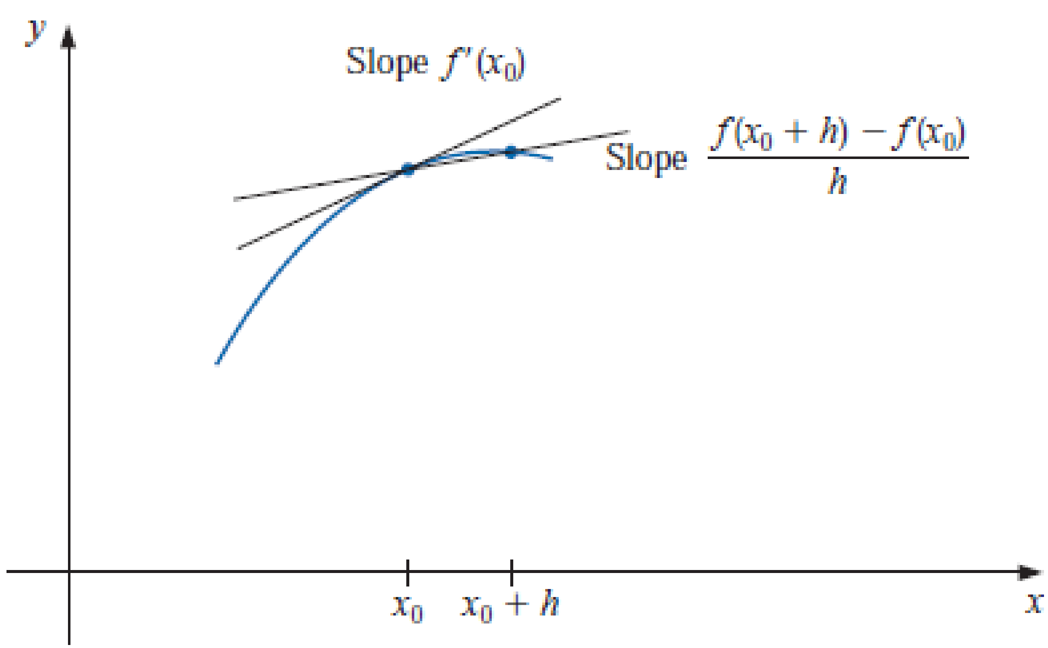
$$f'(x) \approx \frac{f(x_0+h)-f(x_0)}{h}.$$

One difficulty with this formula is that we have no information about $D_x f''(\xi(x))$, so the truncation error cannot be estimated. When x is x_0, however, the coefficient of $D_x f''(\xi(x))$ is 0, and the formula simplifies to

$$f'(x_0) = \frac{f(x_0+h)-f(x_0)}{h} - \frac{h}{2} f''(\xi). \tag{4.1}$$

For small values of h, the difference quotient $[f(x_0+h) - f(x_0)]/h$ can be used to approximate $f'(x_0)$ with an error bounded by $M|h|/2$, where M is a bound on $|f''(x)|$ for x between x_0 and $x_0 + h$. This formula is known as the **forward-difference formula** if $h > 0$ (see Figure 4.1) and the **backward-difference formula** if $h < 0$.

Figure 4.1



Example 1 Use the forward-difference formula to approximate the derivative of $f(x) = \ln x$ at $x_0 = 1.8$ using $h = 0.1$, $h = 0.05$, and $h = 0.01$, and determine bounds for the approximation errors.

Solution The forward-difference formula

$$\frac{f(1.8+h) - f(1.8)}{h}$$

with $h = 0.1$ gives

$$\frac{\ln 1.9 - \ln 1.8}{0.1} = \frac{0.64185389 - 0.58778667}{0.1} = 0.5406722.$$

Because $f''(x) = -1/x^2$ and $1.8 < \xi < 1.9$, a bound for this approximation error is

$$\frac{|hf''(\xi)|}{2} = \frac{|h|}{2\xi^2} < \frac{0.1}{2(1.8)^2} = 0.0154321.$$

The approximation and error bounds when $h = 0.05$ and $h = 0.01$ are found in a similar manner and the results are shown in Table 4.1.

Table 4.1

h	$f(1.8+h)$	$\frac{f(1.8+h) - f(1.8)}{h}$	$\frac{\|h\|}{2(1.8)^2}$
0.1	0.64185389	0.5406722	0.0154321
0.05	0.61518564	0.5479795	0.0077160
0.01	0.59332685	0.5540180	0.0015432

Since $f'(x) = 1/x$, the exact value of $f'(1.8)$ is $0.55\overline{5}$, and in this case the error bounds are quite close to the true approximation error. ■

To obtain general derivative approximation formulas, suppose that $\{x_0, x_1, \ldots, x_n\}$ are $(n+1)$ distinct numbers in some interval I and that $f \in C^{n+1}(I)$. From Theorem 3.3 on page 112,

$$f(x) = \sum_{k=0}^{n} f(x_k)L_k(x) + \frac{(x-x_0)\cdots(x-x_n)}{(n+1)!} f^{(n+1)}(\xi(x)),$$

for some $\xi(x)$ in I, where $L_k(x)$ denotes the kth Lagrange coefficient polynomial for f at $x_0, x_1, \ldots, x_n$. Differentiating this expression gives

$$f'(x) = \sum_{k=0}^{n} f(x_k)L_k'(x) + D_x\left[\frac{(x-x_0)\cdots(x-x_n)}{(n+1!)}\right] f^{(n+1)}(\xi(x))$$

$$+ \frac{(x-x_0)\cdots(x-x_n)}{(n+1)!} D_x[f^{(n+1)}(\xi(x))].$$

We again have a problem estimating the truncation error unless x is one of the numbers x_j. In this case, the term multiplying $D_x[f^{(n+1)}(\xi(x))]$ is 0, and the formula becomes

$$f'(x_j) = \sum_{k=0}^{n} f(x_k)L_k'(x_j) + \frac{f^{(n+1)}(\xi(x_j))}{(n+1)!} \prod_{\substack{k=0\\k\neq j}}^{n} (x_j - x_k), \tag{4.2}$$

which is called an **$(n+1)$-point formula** to approximate $f'(x_j)$.

In general, using more evaluation points in Eq. (4.2) produces greater accuracy, although the number of functional evaluations and growth of round-off error discourages this somewhat. The most common formulas are those involving three and five evaluation points.

We first derive some useful three-point formulas and consider aspects of their errors. Because

$$L_0(x) = \frac{(x - x_1)(x - x_2)}{(x_0 - x_1)(x_0 - x_2)}, \quad \text{we have} \quad L_0'(x) = \frac{2x - x_1 - x_2}{(x_0 - x_1)(x_0 - x_2)}.$$

Similarly,

$$L_1'(x) = \frac{2x - x_0 - x_2}{(x_1 - x_0)(x_1 - x_2)} \quad \text{and} \quad L_2'(x) = \frac{2x - x_0 - x_1}{(x_2 - x_0)(x_2 - x_1)}.$$

Hence, from Eq. (4.2),

$$f'(x_j) = f(x_0)\left[\frac{2x_j - x_1 - x_2}{(x_0 - x_1)(x_0 - x_2)}\right] + f(x_1)\left[\frac{2x_j - x_0 - x_2}{(x_1 - x_0)(x_1 - x_2)}\right]$$

$$+ f(x_2)\left[\frac{2x_j - x_0 - x_1}{(x_2 - x_0)(x_2 - x_1)}\right] + \frac{1}{6} f^{(3)}(\xi_j) \prod_{\substack{k=0 \\ k \neq j}}^{2} (x_j - x_k), \tag{4.3}$$

for each $j = 0, 1, 2$, where the notation ξ_j indicates that this point depends on x_j.

Three-Point Formulas

The formulas from Eq. (4.3) become especially useful if the nodes are equally spaced, that is, when

$$x_1 = x_0 + h \quad \text{and} \quad x_2 = x_0 + 2h, \quad \text{for some } h \neq 0.$$

We will assume equally-spaced nodes throughout the remainder of this section.

Using Eq. (4.3) with $x_j = x_0, x_1 = x_0 + h$, and $x_2 = x_0 + 2h$ gives

$$f'(x_0) = \frac{1}{h}\left[-\frac{3}{2}f(x_0) + 2f(x_1) - \frac{1}{2}f(x_2)\right] + \frac{h^2}{3}f^{(3)}(\xi_0).$$

Doing the same for $x_j = x_1$ gives

$$f'(x_1) = \frac{1}{h}\left[-\frac{1}{2}f(x_0) + \frac{1}{2}f(x_2)\right] - \frac{h^2}{6}f^{(3)}(\xi_1),$$

and for $x_j = x_2$,

$$f'(x_2) = \frac{1}{h}\left[\frac{1}{2}f(x_0) - 2f(x_1) + \frac{3}{2}f(x_2)\right] + \frac{h^2}{3}f^{(3)}(\xi_2).$$

Since $x_1 = x_0 + h$ and $x_2 = x_0 + 2h$, these formulas can also be expressed as

$$f'(x_0) = \frac{1}{h}\left[-\frac{3}{2}f(x_0) + 2f(x_0+h) - \frac{1}{2}f(x_0+2h)\right] + \frac{h^2}{3}f^{(3)}(\xi_0),$$

$$f'(x_0+h) = \frac{1}{h}\left[-\frac{1}{2}f(x_0) + \frac{1}{2}f(x_0+2h)\right] - \frac{h^2}{6}f^{(3)}(\xi_1),$$

and

$$f'(x_0+2h) = \frac{1}{h}\left[\frac{1}{2}f(x_0) - 2f(x_0+h) + \frac{3}{2}f(x_0+2h)\right] + \frac{h^2}{3}f^{(3)}(\xi_2).$$

As a matter of convenience, the variable substitution x_0 for $x_0 + h$ is used in the middle equation to change this formula to an approximation for $f'(x_0)$. A similar change, x_0 for $x_0 + 2h$, is used in the last equation. This gives three formulas for approximating $f'(x_0)$:

$$f'(x_0) = \frac{1}{2h}[-3f(x_0) + 4f(x_0 + h) - f(x_0 + 2h)] + \frac{h^2}{3}f^{(3)}(\xi_0),$$

$$f'(x_0) = \frac{1}{2h}[-f(x_0 - h) + f(x_0 + h)] - \frac{h^2}{6}f^{(3)}(\xi_1),$$

and

$$f'(x_0) = \frac{1}{2h}[f(x_0 - 2h) - 4f(x_0 - h) + 3f(x_0)] + \frac{h^2}{3}f^{(3)}(\xi_2).$$

Finally, note that the last of these equations can be obtained from the first by simply replacing h with $-h$, so there are actually only two formulas:

Three-Point Endpoint Formula

- $$f'(x_0) = \frac{1}{2h}[-3f(x_0) + 4f(x_0+h) - f(x_0+2h)] + \frac{h^2}{3}f^{(3)}(\xi_0), \tag{4.4}$$

where ξ_0 lies between x_0 and $x_0 + 2h$.

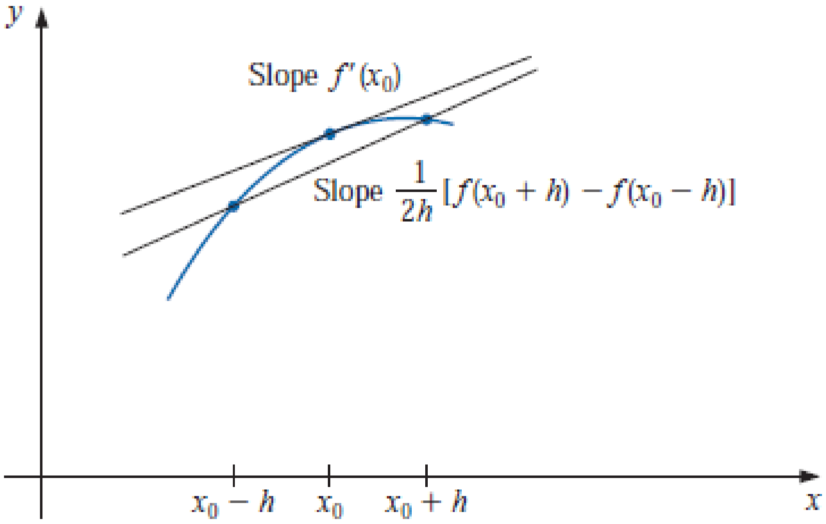
Three-Point Midpoint Formula

- $$f'(x_0) = \frac{1}{2h}[f(x_0+h) - f(x_0-h)] - \frac{h^2}{6}f^{(3)}(\xi_1), \tag{4.5}$$

where ξ_1 lies between $x_0 - h$ and $x_0 + h$.

Although the errors in both Eq. (4.4) and Eq. (4.5) are $O(h^2)$, the error in Eq. (4.5) is approximately half the error in Eq. (4.4). This is because Eq. (4.5) uses data on both sides of x_0 and Eq. (4.4) uses data on only one side. Note also that f needs to be evaluated at only two points in Eq. (4.5), whereas in Eq. (4.4) three evaluations are needed. Figure 4.2 on page 178 gives an illustration of the approximation produced from Eq. (4.5). The approximation in Eq. (4.4) is useful near the ends of an interval, because information about f outside the interval may not be available.

Figure 4.2



Five-Point Formulas

The methods presented in Eqs. (4.4) and (4.5) are called **three-point formulas** (even though the third point $f(x_0)$ does not appear in Eq. (4.5)). Similarly, there are **five-point formulas** that involve evaluating the function at two additional points. The error term for these formulas is $O(h^4)$. One common five-point formula is used to determine approximations for the derivative at the midpoint.

Five-Point Midpoint Formula

- $$f'(x_0) = \frac{1}{12h}[f(x_0 - 2h) - 8f(x_0 - h) + 8f(x_0 + h) - f(x_0 + 2h)] + \frac{h^4}{30}f^{(5)}(\xi), \tag{4.6}$$

  where ξ lies between $x_0 - 2h$ and $x_0 + 2h$.

The derivation of this formula is considered in Section 4.2. The other five-point formula is used for approximations at the endpoints.

Five-Point Endpoint Formula

- $$f'(x_0) = \frac{1}{12h}[-25f(x_0) + 48f(x_0 + h) - 36f(x_0 + 2h) + 16f(x_0 + 3h) - 3f(x_0 + 4h)] + \frac{h^4}{5}f^{(5)}(\xi), \tag{4.7}$$

  where ξ lies between x_0 and $x_0 + 4h$.

Left-endpoint approximations are found using this formula with $h > 0$ and right-endpoint approximations with $h < 0$. The five-point endpoint formula is particularly useful for the clamped cubic spline interpolation of Section 3.5.

Example 2

Values for $f(x) = xe^x$ are given in Table 4.2. Use all the applicable three-point and five-point formulas to approximate $f'(2.0)$.

Table 4.2

x	$f(x)$
1.8	10.889365
1.9	12.703199
2.0	14.778112
2.1	17.148957
2.2	19.855030

$$f'(x_0) = \frac{1}{2h}[-3f(x_0) + 4f(x_0 + h) - f(x_0 + 2h)] + \frac{h^2}{3} f^{(3)}(\xi_0), \quad (4.4)$$

$$f'(x_0) = \frac{1}{2h}[f(x_0 + h) - f(x_0 - h)] - \frac{h^2}{6} f^{(3)}(\xi_1), \quad (4.5)$$

$$f'(x_0) = \frac{1}{12h}[f(x_0 - 2h) - 8f(x_0 - h) + 8f(x_0 + h) - f(x_0 + 2h)] + \frac{h^4}{30} f^{(5)}(\xi), \quad (4.6)$$

Solution The data in the table permit us to find four different three-point approximations. We can use the endpoint formula (4.4) with $h = 0.1$ or with $h = -0.1$, and we can use the midpoint formula (4.5) with $h = 0.1$ or with $h = 0.2$.

Using the endpoint formula (4.4) with $h = 0.1$ gives

$$\frac{1}{0.2}[-3f(2.0) + 4f(2.1) - f(2.2] = 5[-3(14.778112) + 4(17.148957) - 19.855030)] = 22.032310,$$

and with $h = -0.1$ gives 22.054525.

Using the midpoint formula (4.5) with $h = 0.1$ gives

$$\frac{1}{0.2}[f(2.1) - f(1.9)] = 5(17.148957 - 12.7703199) = 22.228790,$$

and with $h = 0.2$ gives 22.414163.

The only five-point formula for which the table gives sufficient data is the midpoint formula (4.6) with $h = 0.1$. This gives

$$\frac{1}{1.2}[f(1.8) - 8f(1.9) + 8f(2.1) - f(2.2)] = \frac{1}{1.2}[10.889365 - 8(12.703199) + 8(17.148957) - 19.855030] = 22.166999$$

If we had no other information we would accept the five-point midpoint approximation using $h = 0.1$ as the most accurate, and expect the true value to be between that approximation and the three-point mid-point approximation that is in the interval [22.166, 22.229].

The true value in this case is $f'(2.0) = (2 + 1)e^2 = 22.167168$, so the approximation errors are actually:

Three-point endpoint with $h = 0.1$: 1.35×10^{-1};

Three-point endpoint with $h = -0.1$: 1.13×10^{-1};

Three-point midpoint with $h = 0.1$: -6.16×10^{-2};

Three-point midpoint with $h = 0.2$: -2.47×10^{-1};

Five-point midpoint with $h = 0.1$: 1.69×10^{-4}. ■

Methods can also be derived to find approximations to higher derivatives of a function using only tabulated values of the function at various points. The derivation is algebraically tedious, however, so only a representative procedure will be presented.

Expand a function f in a third Taylor polynomial about a point x_0 and evaluate at x_0+h and x_0-h. Then

$$f(x_0+h) = f(x_0) + f'(x_0)h + \frac{1}{2}f''(x_0)h^2 + \frac{1}{6}f'''(x_0)h^3 + \frac{1}{24}f^{(4)}(\xi_1)h^4$$

and

$$f(x_0-h) = f(x_0) - f'(x_0)h + \frac{1}{2}f''(x_0)h^2 - \frac{1}{6}f'''(x_0)h^3 + \frac{1}{24}f^{(4)}(\xi_{-1})h^4,$$

where $x_0 - h < \xi_{-1} < x_0 < \xi_1 < x_0 + h$.

If we add these equations, the terms involving $f'(x_0)$ and $-f'(x_0)$ cancel, so

$$f(x_0+h) + f(x_0-h) = 2f(x_0) + f''(x_0)h^2 + \frac{1}{24}[f^{(4)}(\xi_1) + f^{(4)}(\xi_{-1})]h^4.$$

Solving this equation for $f''(x_0)$ gives

$$f''(x_0) = \frac{1}{h^2}[f(x_0-h) - 2f(x_0) + f(x_0+h)] - \frac{h^2}{24}[f^{(4)}(\xi_1) + f^{(4)}(\xi_{-1})]. \qquad (4.8)$$

Suppose $f^{(4)}$ is continuous on $[x_0-h, x_0+h]$. Since $\frac{1}{2}[f^{(4)}(\xi_1) + f^{(4)}(\xi_{-1})]$ is between $f^{(4)}(\xi_1)$ and $f^{(4)}(\xi_{-1})$, the Intermediate Value Theorem implies that a number ξ exists between ξ_1 and ξ_{-1}, and hence in (x_0-h, x_0+h), with

$$f^{(4)}(\xi) = \frac{1}{2}\left[f^{(4)}(\xi_1) + f^{(4)}(\xi_{-1})\right].$$

This permits us to rewrite Eq. (4.8) in its final form.

Second Derivative Midpoint Formula

- $$f''(x_0) = \frac{1}{h^2}[f(x_0 - h) - 2f(x_0) + f(x_0 + h)] - \frac{h^2}{12} f^{(4)}(\xi), \qquad (4.9)$$

  for some ξ, where $x_0 - h < \xi < x_0 + h$.

If $f^{(4)}$ is continuous on $[x_0 - h, x_0 + h]$ it is also bounded, and the approximation is $O(h^2)$.

Example 3

Table 4.3

x	$f(x)$
1.8	10.889365
1.9	12.703199
2.0	14.778112
2.1	17.148957
2.2	19.855030

In Example 2 we used the data shown in Table 4.3 to approximate the first derivative of $f(x) = xe^x$ at $x = 2.0$. Use the second derivative formula (4.9) to approximate $f''(2.0)$.

Solution The data permits us to determine two approximations for $f''(2.0)$. Using (4.9) with $h = 0.1$ gives

$$\frac{1}{0.01}[f(1.9) - 2f(2.0) + f(2.1)] = 100[12.703199 - 2(14.778112) + 17.148957]$$
$$= 29.593200,$$

and using (4.9) with $h = 0.2$ gives

$$\frac{1}{0.04}[f(1.8) - 2f(2.0) + f(2.2)] = 25[10.889365 - 2(14.778112) + 19.855030]$$
$$= 29.704275.$$

Because $f''(x) = (x + 2)e^x$, the exact value is $f''(2.0) = 29.556224$. Hence the actual errors are -3.70×10^{-2} and -1.48×10^{-1}, respectively. ■

Round-Off Error Instability

It is particularly important to pay attention to round-off error when approximating derivatives. To illustrate the situation, let us examine the three-point midpoint formula Eq. (4.5),

$$f'(x_0) = \frac{1}{2h}[f(x_0+h) - f(x_0-h)] - \frac{h^2}{6} f^{(3)}(\xi_1),$$

more closely. Suppose that in evaluating $f(x_0+h)$ and $f(x_0-h)$ we encounter round-off errors $e(x_0+h)$ and $e(x_0-h)$. Then our computations actually use the values $\tilde{f}(x_0+h)$ and $\tilde{f}(x_0-h)$, which are related to the true values $f(x_0+h)$ and $f(x_0-h)$ by

$$f(x_0+h) = \tilde{f}(x_0+h) + e(x_0+h) \quad \text{and} \quad f(x_0-h) = \tilde{f}(x_0-h) + e(x_0-h).$$

The total error in the approximation,

$$f'(x_0) - \frac{\tilde{f}(x_0+h) - \tilde{f}(x_0-h)}{2h} = \frac{e(x_0+h) - e(x_0-h)}{2h} - \frac{h^2}{6} f^{(3)}(\xi_1),$$

is due both to round-off error, the first part, and to truncation error. If we assume that the round-off errors $e(x_0 \pm h)$ are bounded by some number $\varepsilon > 0$ and that the third derivative of f is bounded by a number $M > 0$, then

$$\left| f'(x_0) - \frac{\tilde{f}(x_0+h) - \tilde{f}(x_0-h)}{2h} \right| \le \frac{\varepsilon}{h} + \frac{h^2}{6} M.$$

To reduce the truncation error, $h^2M/6$, we need to reduce h. But as h is reduced, the round-off error ε/h grows. In practice, then, it is seldom advantageous to let h be too small, because in that case the round-off error will dominate the calculations.

Illustration Consider using the values in Table 4.4 to approximate $f'(0.900)$, where $f(x) = \sin x$. The true value is $\cos 0.900 = 0.62161$. The formula

$$f'(0.900) \approx \frac{f(0.900 + h) - f(0.900 - h)}{2h},$$

with different values of h, gives the approximations in Table 4.5.

Table 4.4

x	$\sin x$	x	$\sin x$
0.800	0.71736	0.901	0.78395
0.850	0.75128	0.902	0.78457
0.880	0.77074	0.905	0.78643
0.890	0.77707	0.910	0.78950
0.895	0.78021	0.920	0.79560
0.898	0.78208	0.950	0.81342
0.899	0.78270	1.000	0.84147

Table 4.5

h	Approximation to $f'(0.900)$	Error
0.001	0.62500	0.00339
0.002	0.62250	0.00089
0.005	0.62200	0.00039
0.010	0.62150	−0.00011
0.020	0.62150	−0.00011
0.050	0.62140	−0.00021
0.100	0.62055	−0.00106

The optimal choice for h appears to lie between 0.005 and 0.05. We can use calculus to verify (see Exercise 29) that a minimum for

$$e(h) = \frac{\varepsilon}{h} + \frac{h^2}{6}M,$$

occurs at $h = \sqrt[3]{3\varepsilon/M}$, where

$$M = \max_{x\in[0.800,1.00]} |f'''(x)| = \max_{x\in[0.800,1.00]} |\cos x| = \cos 0.8 \approx 0.69671.$$

Because values of f are given to five decimal places, we will assume that the round-off error is bounded by $\varepsilon = 5 \times 10^{-6}$. Therefore, the optimal choice of h is approximately

$$h = \sqrt[3]{\frac{3(0.000005)}{0.69671}} \approx 0.028,$$

which is consistent with the results in Table 4.6. □

In practice, we cannot compute an optimal h to use in approximating the derivative, since we have no knowledge of the third derivative of the function. But we must remain aware that reducing the step size will not always improve the approximation. □

We have considered only the round-off error problems that are presented by the three-point formula Eq. (4.5), but similar difficulties occur with all the differentiation formulas. The reason can be traced to the need to divide by a power of h. As we found in Section 1.2 (see, in particular, Example 3), division by small numbers tends to exaggerate round-off error, and this operation should be avoided if possible. In the case of numerical differentiation, we cannot avoid the problem entirely, although the higher-order methods reduce the difficulty.

As approximation methods, numerical differentiation is *unstable*, since the small values of h needed to reduce truncation error also cause the round-off error to grow. This is the first class of unstable methods we have encountered, and these techniques would be avoided if it were possible. However, in addition to being used for computational purposes, the formulas are needed for approximating the solutions of ordinary and partial-differential equations.

EXERCISE SET 4.1

5. Use the most accurate three-point formula to determine each missing entry in the following tables.

a.

x	$f(x)$	$f'(x)$
1.1	9.025013	
1.2	11.02318	
1.3	13.46374	
1.4	16.44465	

7. The data in Exercise 5 were taken from the following functions. Compute the actual errors in Exercise 5, and find error bounds using the error formulas.

a. $f(x) = e^{2x}$

$$f'(x_0) = \frac{1}{2h}[-3f(x_0) + 4f(x_0+h) - f(x_0+2h)] + \frac{h^2}{3}f^{(3)}(\xi_0), \tag{4.4}$$

$$f'(x_0) = \frac{1}{2h}[f(x_0+h) - f(x_0-h)] - \frac{h^2}{6}f^{(3)}(\xi_1), \tag{4.5}$$

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h	0,1			
x	f(x)	f´(x)	f´(x) exato	erro
1,1	9,025013	17,769705	18,050027	0,280322
1,2	11,02318	22,193635	22,046353	0,147282
1,3	13,46374	27,107350	26,927476	0,179874
1,4	16,44465	32,510850	32,889294	0,378444

4.2 Richardson's Extrapolation

Richardson's extrapolation is used to generate high-accuracy results while using low-order formulas. Although the name attached to the method refers to a paper written by L. F. Richardson and J. A. Gaunt [RG] in 1927, the idea behind the technique is much older. An interesting article regarding the history and application of extrapolation can be found

Extrapolation can be applied whenever it is known that an approximation technique has an error term with a predictable form, one that depends on a parameter, usually the step size h. Suppose that for each number $h \neq 0$ we have a formula $N_1(h)$ that approximates an unknown constant M, and that the truncation error involved with the approximation has the form

$$M - N_1(h) = K_1 h + K_2 h^2 + K_3 h^3 + \cdots,$$

for some collection of (unknown) constants $K_1, K_2, K_3, \ldots$.

The truncation error is $O(h)$, so unless there was a large variation in magnitude among the constants $K_1, K_2, K_3, \ldots,$

$$M - N_1(0.1) \approx 0.1K_1, \quad M - N_1(0.01) \approx 0.01K_1,$$

and, in general, $M - N_1(h) \approx K_1 h$.

The object of extrapolation is to find an easy way to combine these rather inaccurate $O(h)$ approximations in an appropriate way to produce formulas with a higher-order truncation error.

Suppose, for example, we can combine the $N_1(h)$ formulas to produce an $O(h^2)$ approximation formula, $N_2(h)$, for M with

$$M - N_2(h) = \hat{K}_2 h^2 + \hat{K}_3 h^3 + \cdots,$$

for some, again unknown, collection of constants $\hat{K}_2, \hat{K}_3, \ldots$. Then we would have

$$M - N_2(0.1) \approx 0.01\hat{K}_2, \quad M - N_2(0.01) \approx 0.0001\hat{K}_2,$$

and so on. If the constants K_1 and $\hat{K}_2$ are roughly of the same magnitude, then the $N_2(h)$ approximations would be much better than the corresponding $N_1(h)$ approximations. The extrapolation continues by combining the $N_2(h)$ approximations in a manner that produces formulas with $O(h^3)$ truncation error, and so on.

To see specifically how we can generate the extrapolation formulas, consider the $O(h)$ formula for approximating M

$$M = N_1(h) + K_1 h + K_2 h^2 + K_3 h^3 + \cdots. \tag{4.10}$$

The formula is assumed to hold for all positive h, so we replace the parameter h by half its value. Then we have a second $O(h)$ approximation formula

$$M = N_1\left(\frac{h}{2}\right) + K_1\frac{h}{2} + K_2\frac{h^2}{4} + K_3\frac{h^3}{8} + \cdots. \tag{4.11}$$

Subtracting Eq. (4.10) from twice Eq. (4.11) eliminates the term involving K_1 and gives

$$M = N_1\left(\frac{h}{2}\right) + \left[N_1\left(\frac{h}{2}\right) - N_1(h)\right] + K_2\left(\frac{h^2}{2} - h^2\right) + K_3\left(\frac{h^3}{4} - h^3\right) + \cdots. \tag{4.12}$$

Define

$$N_2(h) = N_1\left(\frac{h}{2}\right) + \left[N_1\left(\frac{h}{2}\right) - N_1(h)\right].$$

Then Eq. (4.12) is an $O(h^2)$ approximation formula for M:

$$M = N_2(h) - \frac{K_2}{2}h^2 - \frac{3K_3}{4}h^3 - \cdots. \tag{4.13}$$

Example 1 In Example 1 of Section 4.1 we use the forward-difference method with $h = 0.1$ and $h = 0.05$ to find approximations to $f'(1.8)$ for $f(x) = \ln(x)$. Assume that this formula has truncation error $O(h)$ and use extrapolation on these values to see if this results in a better approximation.

Solution In Example 1 of Section 4.1 we found that

$$\text{with } h = 0.1\text{: } f'(1.8) \approx 0.5406722, \quad \text{and} \quad \text{with } h = 0.05\text{: } f'(1.8) \approx 0.5479795.$$

This implies that

$$N_1(0.1) = 0.5406722 \quad \text{and} \quad N_1(0.05) = 0.5479795.$$

Extrapolating these results gives the new approximation

$$N_2(0.1) = N_1(0.05) + (N_1(0.05) - N_1(0.1)) = 0.5479795 + (0.5479795 - 0.5406722)$$
$$= 0.555287.$$

The $h = 0.1$ and $h = 0.05$ results were found to be accurate to within 1.5×10^{-2} and 7.7×10^{-3}, respectively. Because $f'(1.8) = 1/1.8 = 0.\overline{5}$, the extrapolated value is accurate to within 2.7×10^{-4}. ■

Extrapolation can be applied whenever the truncation error for a formula has the form

$$\sum_{j=1}^{m-1} K_j h^{\alpha_j} + O(h^{\alpha_m}),$$

for a collection of constants K_j and when $\alpha_1 < \alpha_2 < \alpha_3 < \cdots < \alpha_m$. Many formulas used for extrapolation have truncation errors that contain only even powers of h, that is, have the form

$$M = N_1(h) + K_1 h^2 + K_2 h^4 + K_3 h^6 + \cdots . \tag{4.14}$$

The extrapolation is much more effective than when all powers of h are present because the averaging process produces results with errors $O(h^2)$, $O(h^4)$, $O(h^6)$, ..., with essentially no increase in computation, over the results with errors, $O(h)$, $O(h^2)$, $O(h^3)$, ...

Assume that approximation has the form of Eq. (4.14). Replacing h with $h/2$ gives the $O(h^2)$ approximation formula

$$M = N_1\left(\frac{h}{2}\right) + K_1\frac{h^2}{4} + K_2\frac{h^4}{16} + K_3\frac{h^6}{64} + \cdots .$$

Subtracting Eq. (4.14) from 4 times this equation eliminates the h^2 term,

$$3M = \left[4N_1\left(\frac{h}{2}\right) - N_1(h)\right] + K_2\left(\frac{h^4}{4} - h^4\right) + K_3\left(\frac{h^6}{16} - h^6\right) + \cdots .$$

Dividing this equation by 3 produces an $O(h^4)$ formula

$$M = \frac{1}{3}\left[4N_1\left(\frac{h}{2}\right) - N_1(h)\right] + \frac{K_2}{3}\left(\frac{h^4}{4} - h^4\right) + \frac{K_3}{3}\left(\frac{h^6}{16} - h^6\right) + \cdots .$$

Defining

$$N_2(h) = \frac{1}{3}\left[4N_1\left(\frac{h}{2}\right) - N_1(h)\right] = N_1\left(\frac{h}{2}\right) + \frac{1}{3}\left[N_1\left(\frac{h}{2}\right) - N_1(h)\right],$$

produces the approximation formula with truncation error $O(h^4)$:

$$M = N_2(h) - K_2\frac{h^4}{4} - K_3\frac{5h^6}{16} + \cdots . \tag{4.15}$$

Now replace h in Eq. (4.15) with $h/2$ to produce a second $O(h^4)$ formula

$$M = N_2\left(\frac{h}{2}\right) - K_2\frac{h^4}{64} - K_3\frac{5h^6}{1024} - \cdots .$$

Subtracting Eq. (4.15) from 16 times this equation eliminates the h^4 term and gives

$$15M = \left[16N_2\left(\frac{h}{2}\right) - N_2(h)\right] + K_3\frac{15h^6}{64} + \cdots .$$

Dividing this equation by 15 produces the new $O(h^6)$ formula

$$M = \frac{1}{15}\left[16N_2\left(\frac{h}{2}\right) - N_2(h)\right] + K_3\frac{h^6}{64} + \cdots .$$

We now have the $O(h^6)$ approximation formula

$$N_3(h) = \frac{1}{15}\left[16N_2\left(\frac{h}{2}\right) - N_2(h)\right] = N_2\left(\frac{h}{2}\right) + \frac{1}{15}\left[N_2\left(\frac{h}{2}\right) - N_2(h)\right].$$

Continuing this procedure gives, for each $j = 2, 3, \ldots$, the $O(h^{2j})$ approximation

$$N_j(h) = N_{j-1}\left(\frac{h}{2}\right) + \frac{N_{j-1}(h/2) - N_{j-1}(h)}{4^{j-1} - 1}.$$

Table 4.6 shows the order in which the approximations are generated when

$$M = N_1(h) + K_1 h^2 + K_2 h^4 + K_3 h^6 + \cdots. \tag{4.16}$$

It is conservatively assumed that the true result is accurate at least to within the agreement of the bottom two results in the diagonal, in this case, to within $|N_3(h) - N_4(h)|$.

Table 4.6

$O(h^2)$	$O(h^4)$	$O(h^6)$	$O(h^8)$
1: $N_1(h)$			
2: $N_1(\frac{h}{2})$	**3:** $N_2(h)$		
4: $N_1(\frac{h}{4})$	**5:** $N_2(\frac{h}{2})$	**6:** $N_3(h)$	
7: $N_1(\frac{h}{8})$	**8:** $N_2(\frac{h}{4})$	**9:** $N_3(\frac{h}{2})$	**10:** $N_4(h)$

Example 2 Taylor's theorem can be used to show that centered-difference formula in Eq. (4.5) to approximate $f'(x_0)$ can be expressed with an error formula:

$$f'(x_0) = \frac{1}{2h}[f(x_0+h) - f(x_0-h)] - \frac{h^2}{6}f'''(x_0) - \frac{h^4}{120}f^{(5)}(x_0) - \cdots.$$

Find approximations of order $O(h^2)$, $O(h^4)$, and $O(h^6)$ for $f'(2.0)$ when $f(x) = xe^x$ and $h = 0.2$.

$O(h^2)$ $O(h^4)$ $O(h^6)$

$N_1(h)$ $N_1\left(\frac{h}{2}\right)$ $N_2(h) = \frac{1}{3}\left[4N_1\left(\frac{h}{2}\right) - N_1(h)\right]$ $N_3(h) = \frac{1}{15}\left[16N_2\left(\frac{h}{2}\right) - N_2(h)\right]$

$N_2\left(\frac{h}{2}\right)$

MAP2220

Solution The constants $K_1 = -f'''(x_0)/6$, $K_2 = -f^{(5)}(x_0)/120, \cdots$, are not likely to be known, but this is not important. We only need to know that these constants exist in order to apply extrapolation.

We have the $O(h^2)$ approximation

$$f'(x_0) = N_1(h) - \frac{h^2}{6} f'''(x_0) - \frac{h^4}{120} f^{(5)}(x_0) - \cdots, \tag{4.17}$$

where

$$N_1(h) = \frac{1}{2h}[f(x_0 + h) - f(x_0 - h)].$$

This gives us the first $O(h^2)$ approximations

$$N_1(0.2) = \frac{1}{0.4}[f(2.2) - f(1.8)] = 2.5(19.855030 - 10.889365) = 22.414160,$$

and

$$N_1(0.1) = \frac{1}{0.2}[f(2.1) - f(1.9)] = 5(17.148957 - 12.703199) = 22.228786.$$

Combining these to produce the first $O(h^4)$ approximation gives

$$\begin{aligned} N_2(0.2) &= N_1(0.1) + \frac{1}{3}(N_1(0.1) - N_1(0.2)) \\ &= 22.228786 + \frac{1}{3}(22.228786 - 22.414160) = 22.166995. \end{aligned}$$

To determine an $O(h^6)$ formula we need another $O(h^4)$ result, which requires us to find the third $O(h^2)$ approximation

$$N_1(0.05) = \frac{1}{0.1}[f(2.05) - f(1.95)] = 10(15.924197 - 13.705941) = 22.182564.$$

We can now find the $O(h^4)$ approximation

$$N_2(0.1) = N_1(0.05) + \frac{1}{3}(N_1(0.05) - N_1(0.1))$$

$$= 22.182564 + \frac{1}{3}(22.182564 - 22.228786) = 22.167157.$$

and finally the $O(h^6)$ approximation

$$N_3(0.2) = N_2(0.1) + \frac{1}{15}(N_2(0.1) - N_1(0.2))$$

$$= 22.167157 + \frac{1}{15}(22.167157 - 22.166995) = 22.167168.$$

We would expect the final approximation to be accurate to at least the value 22.167 because the $N_2(0.2)$ and $N_3(0.2)$ give this same value. In fact, $N_3(0.2)$ is accurate to all the listed digits. ■

In Section 4.1, we discussed both three- and five-point methods for approximating $f'(x_0)$ given various functional values of f. The three-point methods were derived by differentiating a Lagrange interpolating polynomial for f. The five-point methods can be obtained in a similar manner, but the derivation is tedious. Extrapolation can be used to more easily derive these formulas, as illustrated below.

Illustration

Suppose we expand the function f in a fourth Taylor polynomial about x_0. Then

$$f(x) = f(x_0) + f'(x_0)(x - x_0) + \frac{1}{2}f''(x_0)(x - x_0)^2 + \frac{1}{6}f'''(x_0)(x - x_0)^3 + \frac{1}{24}f^{(4)}(x_0)(x - x_0)^4 + \frac{1}{120}f^{(5)}(\xi)(x - x_0)^5,$$

for some number ξ between x and x_0. Evaluating f at $x_0 + h$ and $x_0 - h$ gives

$$f(x_0 + h) = f(x_0) + f'(x_0)h + \frac{1}{2}f''(x_0)h^2 + \frac{1}{6}f'''(x_0)h^3 + \frac{1}{24}f^{(4)}(x_0)h^4 + \frac{1}{120}f^{(5)}(\xi_1)h^5 \tag{4.18}$$

and

$$f(x_0 - h) = f(x_0) - f'(x_0)h + \frac{1}{2}f''(x_0)h^2 - \frac{1}{6}f'''(x_0)h^3 + \frac{1}{24}f^{(4)}(x_0)h^4 - \frac{1}{120}f^{(5)}(\xi_2)h^5, \tag{4.19}$$

where $x_0 - h < \xi_2 < x_0 < \xi_1 < x_0 + h$.

Subtracting Eq. (4.19) from Eq. (4.18) gives a new approximation for $f'(x)$.

$$f(x_0+h) - f(x_0-h) = 2hf'(x_0) + \frac{h^3}{3}f'''(x_0) + \frac{h^5}{120}[f^{(5)}(\xi_1) + f^{(5)}(\xi_2)], \quad (4.20)$$

which implies that

$$f'(x_0) = \frac{1}{2h}[f(x_0+h) - f(x_0-h)] - \frac{h^2}{6}f'''(x_0) - \frac{h^4}{240}[f^{(5)}(\xi_1) + f^{(5)}(\xi_2)].$$

If $f^{(5)}$ is continuous on $[x_0-h, x_0+h]$, the Intermediate Value Theorem 1.11 implies that a number $\tilde{\xi}$ in (x_0-h, x_0+h) exists with

$$f^{(5)}(\tilde{\xi}) = \frac{1}{2}\left[f^{(5)}(\xi_1) + f^{(5)}(\xi_2)\right].$$

As a consequence,we have the $O(h^2)$ approximation

$$f'(x_0) = \frac{1}{2h}[f(x_0+h) - f(x_0-h)] - \frac{h^2}{6}f'''(x_0) - \frac{h^4}{120}f^{(5)}(\tilde{\xi}). \quad (4.21)$$

Although the approximation in Eq. (4.21) is the same as that given in the three-point formula in Eq. (4.5), the unknown evaluation point occurs now in $f^{(5)}$, rather than in f'''. Extrapolation takes advantage of this by first replacing h in Eq. (4.21) with $2h$ to give the new formula

$$f'(x_0) = \frac{1}{4h}[f(x_0+2h) - f(x_0-2h)] - \frac{4h^2}{6}f'''(x_0) - \frac{16h^4}{120}f^{(5)}(\hat{\xi}), \quad (4.22)$$

where $\hat{\xi}$ is between x_0-2h and x_0+2h.

Multiplying Eq. (4.21) by 4 and subtracting Eq. (4.22) produces

$$3f'(x_0) = \frac{2}{h}[f(x_0+h) - f(x_0-h)] - \frac{1}{4h}[f(x_0+2h) - f(x_0-2h)]$$
$$- \frac{h^4}{30}f^{(5)}(\tilde{\xi}) + \frac{2h^4}{15}f^{(5)}(\hat{\xi}).$$

Even if $f^{(5)}$ is continuous on $[x_0 - 2h, x_0 + 2h]$, the Intermediate Value Theorem 1.11 cannot be applied as we did to derive Eq. (4.21) because here we have the *difference* of terms involving $f^{(5)}$. However, an alternative method can be used to show that $f^{(5)}(\tilde{\xi})$ and $f^{(5)}(\hat{\xi})$ can still be replaced by a common value $f^{(5)}(\xi)$. Assuming this and dividing by 3 produces the five-point midpoint formula Eq. (4.6) that we saw in Section 4.1

$$f'(x_0) = \frac{1}{12h}[f(x_0-2h) - 8f(x_0-h) + 8f(x_0+h) - f(x_0+2h)] + \frac{h^4}{30}f^{(5)}(\xi). \quad \square$$

Other formulas for first and higher derivatives can be derived in a similar manner. See, for example, Exercise 8.

The technique of extrapolation is used throughout the text. The most prominent applications occur in approximating integrals in Section 4.5 and for determining approximate solutions to differential equations in Section 5.8.

4 Numerical Differentiation and Integration 173

~~4.1 Numerical Differentiation 174~~

~~4.2 Richardson's Extrapolation 185~~

4.3 Elements of Numerical Integration 193

4.4 Composite Numerical Integration 203

4.5 Romberg Integration 213

4.6 Adaptive Quadrature Methods 220

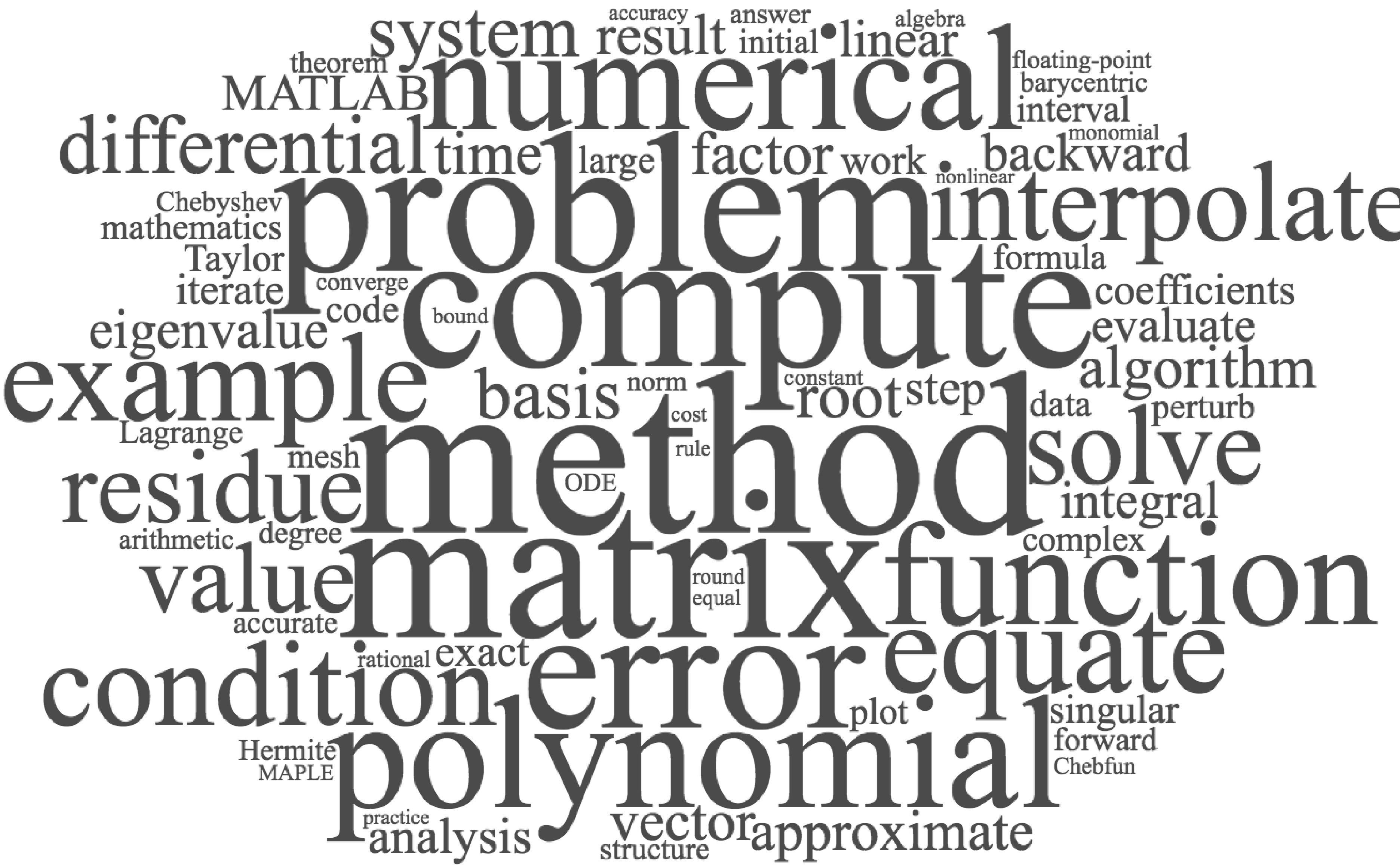
4.7 Gaussian Quadrature 228

4.8 Multiple Integrals 235

4.9 Improper Integrals 250

4.10 Survey of Methods and Software 256

MAP2220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formula
iterate
converge
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coefficients
code
bound
eigenvalue
evaluate
example
algorithm
basis
norm
constant
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perturb
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Lagrange
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